

THE TOTAL RISK INTEGRATED METHODOLOGY
IMPLEMENTATION OF THE TRIM CONCEPTUAL DESIGN
THROUGH THE TRIM.FaTE MODULE
A STATUS REPORT

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Disclaimer

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List of Acronyms

B(a)P	benzo(a)pyrene
CAA	Clean Air Act of 1990
CalTOX	California Department of Toxic Substance Control's Multimedia Risk Computerized Model
CRARM	Presidential/Congressional Commission on Risk Assessment and Risk Management
DOE	U.S. Department of Energy
DTSC	Department of Toxic Substance Control
EPA	U.S. Environmental Protection Agency
FY	fiscal year
g/day	grams per day
GI	gastrointestinal
GIS	Geographic Information System
HAP	hazardous air pollutant
IEM2	Indirect Exposure Methodology
ISMCM	Integrated Spatial Multimedia Compartmental Model
kg/m ² /day	kilograms per square meter per day
km	kilometer
LSODE	Livermore Solver for Ordinary Differential Equation
m/s	meters per second
MCM	Multimedia Compartment Model
MEI	maximally exposed individual
MEPAS	Multimedia Environmental Pollutant Assessment System
µg/kg	micrograms per kilogram
µg/L	micrograms per liter
NAAQS	National Ambient Air Quality Standards
NAS	National Academy of Science
NRC	National Research Council
OAQPS	Office of Air Quality Planning and Standards
P1	Prototype 1
P2	Prototype 2
P3	Prototype 3
P4	Prototype 4
PAH	polycyclic aromatic hydrocarbon
PBPK	physiologically-based pharmacokinetic
PC	personal computer

List of Acronyms (Continued)

SAB	Science Advisory Board
SMCM	Spatial Multimedia Compartment Model
TRIM	Total Risk Integrated Methodology
TRIM.FaTE	TRIM Environmental Fate, Transport, and Exposure Model

1.0 Introduction

The Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency (EPA) is responsible for the evaluation of health risks associated with air pollutants and for the regulation of those pollutants, if needed. To date, OAQPS has not consistently estimated multimedia impacts of air pollutants and has used distinctly different methodologies to estimate risks from hazardous air pollutants (HAP) and criteria air pollutants. While numerous models exist for use in risk assessment, there is no one model or modeling system which meets the needs of OAQPS. As a result, OAQPS is developing the Total Risk Integrated Methodology (TRIM), a multimedia, time-series simulation modeling system for the assessment of human and ecological risks resulting from hazardous and criteria air pollutants. TRIM represents an improved risk assessment tool which:

- Meets the requirements of the Clean Air Act of 1990 (CAA).
- Meets the scientific requirements/capabilities identified by the National Academy of Sciences (NAS), the Presidential/Congressional Commission on Risk Assessment and Risk Management (CRARM), and the EPA.

TRIM will provide a framework that is scientifically defensible, flexible, and user-friendly, for characterizing human health and ecological risk and exposure to hazardous and criteria air pollutants.

The purpose of this report is to summarize the work performed during the first developmental phase of TRIM. The first phase included the conceptualization of TRIM and the implementation of the TRIM conceptual approach through the development of the first TRIM module, the environmental fate, transport, and exposure module, called TRIM.FaTE. TRIM.FaTE development focused on defining the mathematical structure of the module and initial testing and evaluation of these concepts. This report provides detailed information about the overall structure of TRIM and the development of the TRIM.FaTE module. The detailed technical information (mathematical derivations, data inputs, justifications) supporting the testing and implementation is provided in a separate document entitled *The Total Risk Integrated Methodology: Technical Support Document for TRIM.FaTE*¹.

1.1 Clean Air Act Requirements

The CAA contains several provisions that require EPA to evaluate effects to humans and the environment caused by exposure to HAPs and criteria pollutants. In support of the CAA requirements, and in response to recommendations of the NAS and the CRARM, and EPA risk

assessment policies and guidelines, EPA is developing TRIM. TRIM will provide a framework for assessing human health and ecological risks attributable to HAP and criteria pollutants and, thus, will include the capability to assess multimedia contamination (in air, water, soil, food, and indoor environments) and multipathway exposure (via inhalation, ingestion, and absorption exposure routes).

TRIM will be a useful tool for performing risk assessments needed by many CAA programs, including: the Residual Risk Program (Section 112[f]); the Urban Area Source Program (Section 112[k]); the Special Studies (Sections 112[m] and 112[n]); petitions to delist source categories and/or individual HAPs (Sections 112[b][3] and 112[c][9]); and review and setting of the national ambient air quality standards (NAAQS) (Section 109).

1.2 Recommendations for Improving Risk Assessment

The risk assessment tools used by OAQPS must have maximum technical credibility and, therefore, must address the recommendations of the NAS and the CRARM and be consistent with EPA guidance and guidelines for risk and exposure assessment. Some of these recommendations and guidelines are described in the following sections.

1.2.1 National Research Council Report

As required by Section 112(o) of the CAA, the EPA commissioned the National Research Council (NRC) to perform a study of the risk assessment methods used by EPA for the evaluation of HAP. The NRC created the Committee on Risk Assessment of Hazardous Air Pollutants, within the Board on Environmental Studies and Toxicology, to: (1) review the risk assessment methods used by EPA; (2) evaluate methods used for estimating the carcinogenic potency of HAPs; (3) evaluate methods used for estimating human exposures; (4) evaluate risk assessment methods for noncancer health effects for which safe thresholds may not exist; and (5) indicate revisions needed in EPA's risk assessment guidelines. The resulting 1994 NRC report, *Science and Judgment in Risk Assessment*,² outlined the Committee's observations and recommendations.

The NRC Committee observed that several themes that were common to all elements of the risk assessment process also were usually the focal points for criticisms of specific risk assessments. The themes discussed included the use of default assumptions; the lack of available data; the need for a tiered, iterative approach to risk assessment; the need for quantification of uncertainty and variability inherent in the risk assessment process; the assessment of multiple chemical exposures, multiple routes of exposure, and the potential for multiple adverse effects; and the documentation of the steps taken to validate the methodologies used throughout the risk assessment process.

The NRC concluded that EPA should retain its conservative, default-based approach to risk assessment for screening analysis in standard setting. However, the Committee made specific recommendations regarding ways that the process should be improved, including using defaults, and explicitly identifying and better explaining all defaults; developing and using an iterative approach to health risk assessments; and identifying the sources and magnitudes of uncertainty associated with estimates of risk.

1.2.2 CRARM Report

The CRARM was also mandated by Congress, under the CAA, to: (1) assess uses and limitations of risk assessment; (2) evaluate exposure scenarios for risk characterization; (3) determine how to describe and explain uncertainties; (4) enhance strategies for risk-based management decisions; and (5) review the desirability of consistency across federal programs. The CRARM was also asked to make recommendations on the EPA peer review process and to comment on the conclusions of the NRC's *Science and Judgment in Risk Assessment*². The CRARM report³ identified several risk management contexts that may be relevant for a risk assessment, including the consideration of multimedia, multisource, and/or multichemical exposures, as well as multiple risks from different stressors.

The CRARM report recommended that risk assessments should take into consideration genetic and other differences in receptor susceptibility, recognize the spectrum of interindividual variations within the population, and identify subpopulations that are especially susceptible to specific chemical exposures. In addition, CRARM identified the need for exposure assessments to be designed to be commensurate with the needs of the risk management decisions. CRARM also identified the need for more realistic exposure scenarios. The report recommended that screening risk assessments should rely on more representative estimates, such as a maximally exposed actual person, rather than on a hypothetical maximally exposed individual (MEI). Other recommendations included identifying highly exposed populations or subpopulations, and performing ecological risk assessments.

1.2.3 Other Risk Guidance

EPA has prepared numerous guidance on risk assessment and risk assessment methods, starting with the 1986 risk assessment guidelines, which included *Guidelines for Carcinogenic Risk Assessment*⁴, *Guidelines for Mutagenicity Risk Assessment*⁵, *Guidelines for the Health Risk Assessment of Chemical Mixtures*⁶, and *Guidelines for Exposure Assessment*⁷. These guidelines have been subsequently augmented or revised. Most notably, the EPA has revised guidelines for exposure assessment and has prepared new guidance on risk characterization and probabilistic analysis.

EPA's 1995 *Policy for Risk Characterization*⁸ stresses the importance of risk characterization and calls for all risk characterizations prepared at EPA, or submitted to EPA by outside parties, to be done in a manner that is transparent, clear, reasonable, and consistent with other risk characterizations of similar scope prepared across programs in the Agency.

Both the revised *Guidelines for Exposure Assessment*⁷ and *Policy for Use of Probabilistic Risk Analysis in Risk Assessment*⁹ emphasize a distributional or probabilistic approach toward risk assessment, moving away from the deterministic "point estimate" approach. *Guidelines for Exposure Assessment*⁷ provides several descriptors of exposure and risk aimed at presenting a fuller picture of risk that corresponds to the range of different exposure conditions encountered by various individuals and populations exposed to environmental chemicals. The guidelines recommend that central tendency and high-end exposures be characterized, as well as the distribution of exposures and risks among the exposed population. EPA's *Policy for Use of Probabilistic Risk Analysis in Risk Assessment*⁹ emphasizes the use of probabilistic analysis to generate distributional estimates of risks to provide more information to the risk manager. In response to the need for probabilistic analysis in risk assessment (also called for by NAS and CRARM), EPA has prepared *Guiding Principles for Monte Carlo Analysis*¹⁰, which establishes principles for how such analyses should be included in risk assessments.

The 1997 EPA document *Guidance on Cumulative Risk Assessment*¹¹ discusses the Agency's move to an emphasis on a more broadly based approach to risk assessment, characterized by greater consideration of multiple endpoints, sources, pathways, and routes of exposure, as well as flexibility in achieving goals and holistic reduction of risk, among other features. Cumulative risk assessments are integrated assessments potentially involving multiple pollutants in several media that may cause a variety of adverse effects to humans and other biota, or even to ecosystems and their processes and functions. In planning a risk assessment, the guidance recommends defining the dimensions of the assessment, including the characteristics of the population at risk. These characteristics include individuals or sensitive subgroups that may be highly susceptible to risks from stressors or groups of stressors.

1.3 The Need for an Improved Risk Assessment Tool: TRIM

Based on the recommendations of the NAS and the CRARM, as well as the current EPA guidelines and policies, in combination with the CAA requirements, OAQPS recognized the need for improvements in risk and exposure assessment tools. OAQPS currently has a variety of tools for HAP and criteria air pollutant exposure and risk assessments, though several significant features were determined to be lacking in the current models. To be consistent with the recommendations of the NAS and the CRARM, as well as EPA guidelines and policies, OAQPS

needs modeling tools that: (1) have multimedia assessment capabilities; (2) have ecosystem risk and exposure modeling capabilities; (3) can perform multi-pollutant assessments (e.g., assess mixtures of pollutants, track chemical transformations); (4) can explicitly address uncertainty and variability; and (5) are readily available and user-friendly, so that they can be used by EPA, state and local agencies, and other stakeholders. OAQPS also needs HAP exposure and risk models that adequately estimate temporal and spatial patterns of exposures and that maintain mass-balance. While many current OAQPS criteria air pollutant exposure and risk models have these advanced features, the HAP models do not. Finally, OAQPS and others recognize the importance of having modeling tools with the capability to model pollutant uptake, biokinetics, and dose-response for HAPs and criteria air pollutants where possible and relevant.

A risk and exposure assessment model, or set of models, with all of the previously noted features does not exist. Although individual models that perform individual functions do exist, none of these, separately or in combination with other models, provide an integrated system that could function to meet the modeling needs previously described. Therefore, to meet the specific modeling needs of OAQPS, the conceptual framework for TRIM was developed. The TRIM conceptual approach and the modular design of TRIM are described in Chapter 2.0. The fate and transport module has been the focus of the first implementation phase of TRIM's conceptual approach. This multimedia model, TRIM.FaTE, is described in Chapters 3.0 through 6.0 of this report. Future directions for the overall TRIM framework are presented in Chapter 7.0.

2.0 TRIM Conceptual Approach

2.1 Overall Goals and Objectives

The goal in developing TRIM is to create a modeling system, and the components of that system, to appropriately characterize human health and ecological risk and exposure in support of hazardous and criteria air pollutant programs under the CAA. The goal in designing TRIM is to develop a modeling system that is: (1) scientifically defensible, (2) flexible, and (3) user-friendly.

(1) To be scientifically defensible, TRIM will be:

- **Mass-Conserving.** Pollutant mass is conserved, within the system being assessed.
- **Stochastic.** Input data may be represented as ranges or probability distributions rather than point estimates.
- **Able to characterize uncertainty and variability.** Uncertainty and variability in outputs are characterized using stochastic simulation and distributional data.
- **Capable of assessing multiple pollutants, multiple media, and multiple exposure pathways.** Cumulative effects, due to multiple sources and/or multiple pollutants affecting the same target organ or organism, may be estimated; chemical and/or chemical species transformations are tracked.
- **Able to perform iterative analyses.** The user may select the necessary level of analysis, ranging from a screening level to a detailed risk assessment.

(2) To ensure flexibility, TRIM will be:

- **Modular in design.** Only those model components necessary for evaluating the particular pollutants of interest and/or endpoints of interest need to be selected and used.
- **Flexible in temporal and spatial scale.** Risk assessments are possible for a wide range of temporal and spatial scales, including hourly to daily or yearly time frames, temporally, and, spatially, from local scale (10 kilometers [km] or less) to urban scale (approximately 100 km or less), or even greater.
- **Able to assess human and ecological endpoints.** Impacts to humans and/or biota, for individuals and/or populations, may be assessed.

(3) TRIM must also be usable by OAQPS, EPA Regions, states, and stakeholders. Therefore, the goal is to develop a model that will be:

- **Easily accessible.** TRIM will be accessible through a personal computer (PC) and/or via the INTERNET and/or through an EPA model framework (e.g., Models-3).
- **Well-documented.** Detailed instructions for use of the model will be provided through a user's guide, with a focus on the modular aspects of the modeling system and how to specify user options.
- **Clear and transparent.** The graphical user interface will provide transparency and clarity in the model function, and the risk characterization module will provide information on model assumptions, limitations, and uncertainties.

2.2 Model Design

TRIM will provide a framework for assessing human health and ecological risks resulting from multimedia contamination (in air, water, soil, and food) and multipathway exposure (via inhalation, ingestion, and absorption exposure routes) to HAPs and criteria pollutants. TRIM will be a dynamic modeling system that tracks the movement of pollutant mass through a comprehensive system of compartments, providing an inventory of a pollutant throughout the entire system. The compartments will be able to represent possible locations of the pollutant in the physical and biological environments of a defined study area or species. Receptors may move through these compartments for the estimation of exposure. Uptake, biokinetics, and dose-response models may be used to determine dose and health impacts. The model will address uncertainty and variability issues by evaluating a range of parameters.

The goal in developing TRIM is to create a modeling system that is complex enough to appropriately characterize human health and ecological risk and exposure, yet simple enough to be useful in performing risk analyses for use in regulatory decision making. An extremely simple modeling approach may be too restrictive to support risk and exposure assessments across the CAA programs. An extremely complex model may be too difficult to initialize or may require prohibitive amounts of data. The aim of developing TRIM is to suppress the less necessary details and to focus on the processes that have the most significant impact on human health and ecological risk.

For the development of TRIM, existing models and tools will be adopted, where possible. Incorporating existing models or model features into a modeling tool that meets OAQPS needs is preferable since it is the most efficient and cost-effective approach.

As shown in Figure 2-1, TRIM is designed to be modular and will be an assembly of six primary modules. Depending on the user's needs for a particular assessment, it may be possible to use any one or more of these modules for an assessment. The first TRIM module, TRIM.FaTE, accounts for movement of the pollutant mass through the ecosystem and determines the pollutant concentration in media and biota. Exposures will be evaluated within the TRIM Exposure Event Module by tracking small population groups of humans and/or other organisms, referred to as "cohorts," through time and space. Also included in TRIM will be a Pollutant Uptake Module, which will determine the quantity of a pollutant entering an organism during a specific exposure event; a Biokinetics Module, which will determine the quantity of a pollutant delivered to a target organ; and a Dose-Response Module, which will estimate health effects caused by the pollutant quantity delivered to a target organ. The final module of TRIM, the Risk Characterization Module, will present the risk estimates, assumptions, and uncertainties. A brief summary of each module follows.

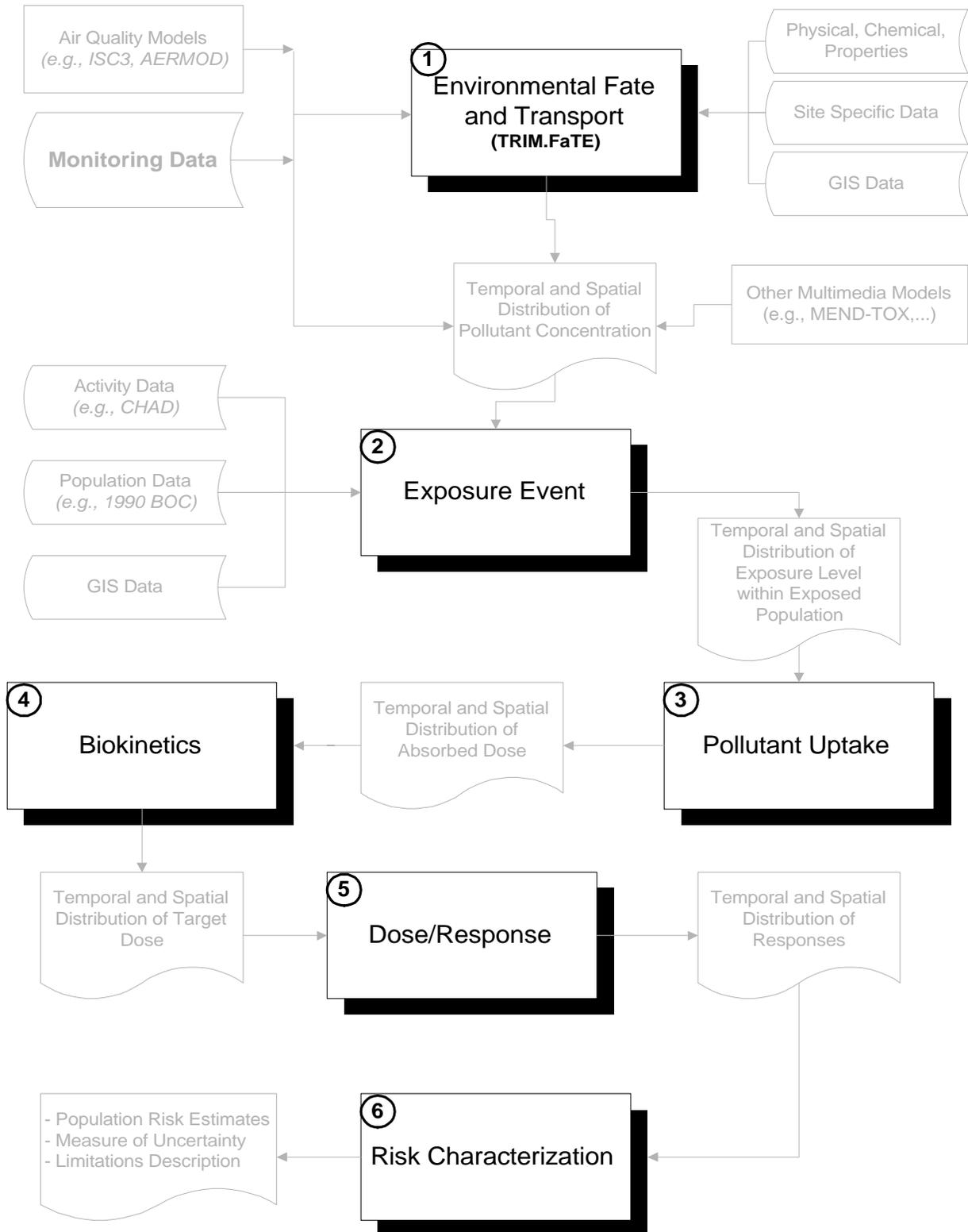
2.2.1 Environmental Fate and Transport (TRIM.FaTE) Module

TRIM.FaTE will estimate pollutant concentrations in multiple environmental media and biota, a capability not currently available in other EPA air exposure models. TRIM.FaTE has been the focus of current development efforts, and a TRIM.FaTE prototype has been developed. This development has produced a library of algorithms that account for transfer of mass throughout an environmental system, data to initialize these algorithms for a test site, and a working prototype. The TRIM.FaTE module will model the movement of pollutant mass over time, through a user-defined, bounded system, which includes both biotic and non-biotic (abiotic) components. Complete details on the TRIM.FaTE module are presented in Chapters 3.0 through 6.0.

2.2.2 Exposure Event Module

The Exposure Event Module will be used to move a cohort of humans or other organisms through locations where exposure can occur according to a specific activity pattern. The development of this module will take place primarily in 1998 and 1999. In a typical application, TRIM.FaTE may be used to provide an inventory of pollutant mass across the ecosystem at selected time intervals (i.e., days, hours). For pollutants believed to exhibit toxicity via direct inhalation exposure only (i.e., those that are not persistent and/or bioaccumulative), monitoring data or air dispersion modeling results may be used in place of data from a fate and transport model. With these pollutant data as inputs, the Exposure Event Module may be used to define

Figure 2-1. Conceptual Overview of TRIM



the movements of a human or other organism, or a population of organisms (e.g., a population of an endangered species). The movements could be defined as an exposure event sequence that corresponds to the time periods modeled by TRIM.FaTE. Each exposure event would place the organism in contact with one or more of the cells in the ecosystem for a specified time interval. For example, a particular event may assign the organism to an air cell and a water cell for specified time intervals (i.e., 1 hour, 1 day). In addition to the location assignments, the event would provide information relating to the potential for exposure, such as respiration rate (air cell) and quantity of water consumed (water cell).

2.2.3 Pollutant Uptake Module

The Pollutant Uptake Module will be used to determine the quantity of a pollutant entering an organism during a specific exposure event. Development of this module will occur in 1999 and 2000 using existing models, where possible. To more accurately estimate dose (and risk) within an exposed population, the Pollutant Uptake Module will use exposure estimates to calculate the uptake of a toxic chemical via inhalation (absorption through the lungs), ingestion (absorption through the gastrointestinal [GI] tract), and dermal exposure (absorption through skin or plant membrane).

2.2.4 Biokinetics Module

The Biokinetics Module will be used to determine the quantity of a pollutant delivered to a target organ. Development of the Biokinetics Module will occur in 1999 and 2000 using existing models, where possible. Since the toxicity of an agent is determined by the concentration of the toxic chemical in the target organ or tissue, and since the concentration in the target organ or tissue depends on the disposition of the chemical (i.e., absorption, distribution, biotransformation, and excretion), accounting for these processes will result in a more accurate estimation of risk. This is the case because the amount of toxic chemical reaching the target organ may be higher or lower than the amount that would be predicted if the chemical were assumed to be uniformly distributed throughout the organism. The Biokinetics Module will use the dose estimates generated by the uptake module to depict the range of target organ doses (and risks) within an exposed population.

2.2.5 Dose-Response Module

The Dose-Response Module will estimate health effects caused by the pollutant quantity delivered to a target organ. Development of the module will occur primarily in 1999 and 2000 using existing models, where possible. A module is desired that can address or apply EPA-verified

health benchmarks, such as cancer slope factors and reference concentrations, to assess risks associated with mixtures, evaluate the impacts of dose-rate on toxicity, and determine the impacts of threshold and non-threshold mechanisms of action.

2.2.6 Risk Characterization Module

The Risk Characterization Module will present the risk estimates, as well as a description of major assumptions, defaults, and uncertainties, from the risk analysis. The Risk Characterization Module will be developed starting in 1998 and continuing into 1999. The results of any risk assessment conducted using the TRIM are intended to support regulatory decision-making. Therefore, it is critical that TRIM provide results in a manner that is meaningful to EPA risk managers. This module will format and present risk estimates and related information in a systematic manner that promotes regulatory decision making and meets the objectives outlined in current EPA guidance and policy. Ideally, this module will present risk assessment information in several formats (e.g., graphics, tables) such that risk managers can best interpret and understand the risk assessment results.

3.0 Conceptual Framework for TRIM.FaTE

An environmental fate, transport, and exposure model is needed by OAQPS to address non-inhalation (indirect) routes of exposure not presently addressed in many current models. TRIM.FaTE has been designed for this reason. TRIM.FaTE is a multimedia chemical mass balance model being developed to assess contaminant transport among environmental compartments (such as air, water, and soil) and link these compartments with ecosystem components. This chapter describes the initial review of multimedia models and explains the rationale for developing TRIM.FaTE. In addition, the overall logic and terminology for TRIM.FaTE for expressing transport and transformation of chemical contaminants in a multimedia environment is provided. This chapter also describes the processes being simulated in TRIM.FaTE, illustrates and discusses the mass balance approach and the resulting system of differential equations for first-order systems, and demonstrates the application of the TRIM mass-balance approach to a simple four-compartment environmental system.

3.1 Review of Existing Tools

The first step in the model development process was to evaluate EPA and non-EPA approaches already existing in the fields of non-inhalation exposure assessment that may meet or contribute to the needs of the TRIM approach. In April 1996, a review of existing models and approaches was undertaken as part of the initial step in the TRIM development effort. The report, entitled *Evaluation of Existing Approaches for Assessing Non-Inhalation Exposure and Risk with Recommendations for Implementing TRIM*¹², examined several multimedia models. Two additional EPA studies^{10,11} conducted in 1997 have updated the 1996 study.

The literature searches identified several models/approaches for multimedia, multipathway modeling for evaluation, including EPA's Indirect Exposure Methodology (IEM2), the California Department of Toxic Substance Control's Multimedia Risk Computerized Model (CalTOX), the Integrated Spatial Multimedia Compartmental Model (ISMCM), and the Multimedia Environmental Pollutant Assessment System (MEPAS).

Efforts to assess human exposure from multiple media date back to the 1950s, when the need to assess human exposure to global fallout led rapidly to a framework that included transport both through and among air, soil, surface water, vegetation, and food chains¹³. Efforts to apply such a framework to non-radioactive organic and inorganic toxic chemicals have been more recent and have not as yet achieved the level of sophistication that exists in the radioecology field. In

response to the need for multimedia models in exposure assessment, a number of multimedia transport and transformation models have recently appeared. Thibodeaux^{14,15} proposed the term “chemodynamics” to describe a set of integrated methods for assessing the cross-media transfers of organic chemicals. The first widely used multimedia compartment modeling for organic chemicals were the “fugacity” models proposed by Mackay^{16,17} and Mackay and Paterson^{18,19}. Cohen and his co-workers applied the concept of multimedia compartment modeling as a screening tool by developing the Multimedia Compartment Model (MCM)²⁰, followed by the Spatial Multimedia Compartment Model (SMCM)²¹, and more recently the ISMCM, which allows for non-uniformity in some compartments. Another multimedia screening model, called GEOTOX²² was one of the earliest multimedia models to explicitly address human exposure. The CalTOX program^{23,24,25} has been developed for the California EPA as a set of spreadsheet models and spreadsheet data sets to assist in assessing human exposures for toxic substances releases in multiple media. More recently, SimpleBOX, Version 2.0²⁶ has been developed for the National Institute of Public Health and the Environment in the Netherlands in order to evaluate the environmental fate of chemicals. Results can be for a level 3 (non-equilibrium, steady state) or quasi-dynamic level 4 (non-equilibrium, non-steady state) system. All phases within the compartments are assumed to be in a state of thermodynamic equilibrium at all times.

A brief summary of each of the multimedia models that were evaluated for its applicability to the TRIM effort follows:

- **Indirect Exposure Methodology (IEM2).** With an interim final document completed in 1990²⁷ and with an addendum completed in 1993²⁸, the IEM incorporates current EPA guidance. Descriptions of the fate and transport, exposure pathways, and dose algorithms are presented in this methodology. This methodology sets out procedures for estimating the indirect (i.e., non-inhalation) human exposures and health risks that can result from the transfer of emitted pollutants to soil, vegetation, and water bodies. The methodology addresses exposures via inhalation; food, water, and soil ingestion; and, dermal contact. There appear to be several shortcomings in the methodology. For example, the methodology, as currently implemented, can be applied only to chemicals that are emitted to the air. This methodology is not a comprehensive environmental audit, but is best regarded as an evolving and emerging process that moves EPA beyond the analysis of potential effects associated with only one medium (air) and exposure pathway (inhalation) to the consideration of other media and exposure pathways. Most importantly, it is crucial in the development of TRIM that a sense of continuity be maintained between the existing (IEM2) and proposed (TRIM) methodologies. IEM2 has undergone extensive scientific review.

The Science Advisory Board (SAB) has identified several major limitations of IEM, which can be useful in focusing efforts in TRIM development. While IEM represents the current EPA guidance on multimedia multipathway modeling, it does not meet the needs of OAQPS. One of the major limitations of IEM is that it consists of a one-way process through a “train” of linked models or algorithms and is based on annual average air concentrations, wet and dry deposition values from air dispersion modeling. As a result, it is not a truly coupled multimedia model and thereby does not have the ability to model “feedback” loops or secondary emissions and cannot provide time-series estimation of media concentrations and concomitant exposure. In addition, the methodology does not provide for flexibility in site-specific applications or in estimating population exposures. Significant site-specific adjustment must be made to allow for spatially tracking differences in concentrations and exposure. Much of the focus is on evaluating specific receptor scenarios (e.g., recreational or subsistence fisher) that may be indicative of high-end or average exposures but does not allow for modeling the range of exposure scenarios within a population. Therefore, IEM cannot estimate population exposure distributions. More recent advances²⁹ have addressed some of these limitations to some degree but have not been fully implemented.

- **California Department of Toxic Substance Control's Multimedia Risk Computerized Model (CalTOX).** First issued in 1993 and updated in 1995, with continual enhancements underway, CalTOX was developed as a spreadsheet model for California's Department of Toxic Substance Control (DTSC), to assist in human health risk assessments that address contaminated soils and the contamination of adjacent air, surface water, sediment, and groundwater. CalTOX consists of two component models: a multimedia transport and transformation (i.e., fate and transport) model, which is based on both conservation of mass and chemical equilibrium; and, a multipathway human exposure model that includes ingestion, inhalation, and dermal uptake exposure routes. CalTOX is a fully mass balancing model and also includes add-ins to quantify uncertainty and variability.

The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of contaminants introduced initially to soil layers or for contaminants released continuously to air, soil, or water. The CalTOX multimedia model is a seven-compartment regional and dynamic multimedia fugacity model. The seven compartments are (1) air, (2) ground surface soil, (3) plants, (4) root-zone soil, (5) the vadose-zone soil below the root zone, (6) surface water, and (7) sediment. The air, surface water, ground surface soil, plants, and sediment compartments are assumed to be in quasi-steady state with the root-zone soil, and vadose-zone soil compartments. Contaminant inventories in the root-zone soil and vadose-soil zone are treated as time-varying state variables. Contaminant concentrations in groundwater are based on the leachate from the vadose-zone soil.

The multipathway exposure model encompasses 23 exposure pathways, which are used to estimate average daily doses within a human population in the vicinity of a

hazardous substances release site. The exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments to contaminant concentrations in the media with which a human population has contact (personal air, tap water, foods, household dusts/soils, etc.). The explicit treatment of differentiating environmental media pollutant concentration and the pollutant concentration to which humans are exposed favorably distinguishes CalTOX from many other exposure models. In addition, all parameter values used as inputs to CalTOX are distributions, described in terms of mean values and a coefficient of variation, rather than as point estimates or plausible upper values such as most other models employ. This stochastic approach allows both sensitivity and uncertainty to be directly incorporated into the model operation. This model does not conserve mass.

As indicated in the literature review reports, the CalTOX model appears to be the most promising existing model for application to the TRIM effort. Several of the mathematical concepts and derivations used by the developers of CalTOX can be directly applied to the TRIM approach. However, CalTOX does have several limitations that prevent it from being entirely imported into the TRIM approach. These limitations result from going beyond intended applications for CalTOX; for example, for landscapes in which there is a large ratio of land area to surface water area, for a limited range of chemicals (e.g., non-ionic organic chemicals in a liquid or gaseous state). As a result, the model does not provide adequate flexibility in environmental settings and chemical classes (e.g., volatile metals such as mercury) to be suitable for OAQPS needs. The most significant of these limitations, in terms of application to TRIM, is the fact that the CalTOX model, as it currently exists, does not allow spatial tracking of a pollutant as is required in the TRIM approach.

- **SimpleBox.** SimpleBOX is a steady-state, non-equilibrium partitioning, mass balance model. It consists of eight compartments, three of which are soils of differing use and properties. It also produces quasi-dynamic (non-steady-state) output by using an external numerical integrator. The model was developed as a regional scale model for the Netherlands, so its default characteristics represent the Netherlands³⁰. SimpleBOX uses the classical concentration concept to compute the mass balance. Its goals are comparable to TRIM to the extent that it simulates regional systems³¹; however, its level of spatial and temporal complexity does not match TRIM's goals.
- **Integrated Spatial Multimedia Compartmental Model (ISMCM).** ISMCM has been under development with the School of Engineering and Applied Science at University of California Los Angeles for the approximately 15 years. A newer version of ISMCM, called MEND-TOX, is currently under evaluation by the EPA's Office of Research and Development National Exposure Research Laboratory.

ISMCM considers all media, biological and non-biological, in one integrated system. ISMCM includes both spatial and compartmental modules to account for complex transport of pollutants through the ecosystem. Assuming mass conservation,

ISMCM is able to predict transport based on a sound mechanistic description of environmental processes, including estimation of intermedia transfer factors. One of the limiting factors with the ISMCM system for use in the TRIM system is that it is not structured to incorporate uncertainty/variability directly into the model operation.

One of the limitations of the ISMCM model within the context of the goals for TRIM (as described in 1995 thesis³²) is the fact that the links and compartments (spatial configuration) of this model are predetermined. ISMCM was apparently not designed from start with the necessary flexibility. Having this flexibility is not a trivial thing to request, if the system is to be fully integrated.

- ***Multimedia Environmental Pollutant Assessment System (MEPAS).*** MEPAS was developed at the U.S. Department of Energy's (DOE) Pacific Northwest Laboratory to assess risks from mixed wastes at DOE facilities. MEPAS is a model that can be run on IBM-compatible PCs. This model consists of single-media transport models linked together under appropriate boundary conditions. The model considers four primary pollutant pathways (groundwater, overland, surface water, and atmospheric) in evaluating human exposure and health effects. The model also contains an exposure and risk module. The model's ability to estimate multipathway risks for chemicals and radionuclides makes it unique. The nature of its algorithms make it a screening tool, rather than a detailed assessment tool. The model is updated periodically and the latest version of MEPAS (Version 3.1) also contains a uncertainty and variability analysis module (SUM)³³. The mathematical design of this model does not include mass balance and could not be integrated into TRIM.

As with IEM2, MEPAS represents a "linked" model system that utilizes a one-way process through a train of models that individually describe a specific environmental process or media. These types of models are not mass conservative and do not allow for appropriate temporal tracking of the pollutants and concomitant exposure.

3.2 The Need for an Improved Fate and Transport Modeling Tool: TRIM.FaTE

Current OAQPS models for hazardous and criteria air pollutants do not address multimedia exposures, and current OAQPS HAP models do not adequately estimate temporal and spatial patterns of exposures. Adopting or incorporating existing models into a tool that meets OAQPS needs represents the most cost-effective approach to developing the tools needed to support regulatory decision making related to hazardous and criteria air pollutants. Based on the OAQPS review of current multimedia models or modeling systems (described in Section 3.1), there is no single model that meets the needs of OAQPS (outlined in Section 1.3 above) and that can be adopted as part of TRIM. Most models are limited in the type of media and environmental processes addressed. No single model can address the broad range of pollutants and environ

mental fate and transport processes anticipated to be encountered by OAQPS in evaluating risks from hazardous and criteria air pollutants. In addition, it is also not likely that one individual model could be developed to address this wide range of concerns. Therefore, the TRIM framework emphasizes a modular design. The lack of a flexible multimedia fate and transport model was identified as a major limitation and has become the focus of the first phase implementation efforts for TRIM.

Current multimedia models can be divided into three basic categories, each with its own advantages and disadvantages: “linked” model systems, fugacity models, and compartmental models. However, the identified limitations were considered critical and, therefore, deemed unacceptable for incorporating such models into TRIM. “Linked” model systems (e.g., IEM2, MEPAS) generally utilize a one-way process through a series of linked models that mathematically describe distinct environmental media or processes (e.g., aquatic environment). These types of models can never be truly mass conserving and cannot address feedback loops and secondary pollutant movement (e.g., revolatilization and transport). Fugacity models (e.g., CalTOX) typically are compartment modes without explicit spatial scale (zero dimensional); thus, they do not provide the ability to spatially track pollutant movement. They are also applicable only to a limited range of chemical classes (e.g., inappropriate to model volatile metals [e.g., mercury]). Compartmental models (e.g., MCM) are also zero dimensional and do not allow for spatial tracking of pollutant movement and concomitant exposures. Spatial compartmental models (e.g., ISMCM) represent the closest current models to an integrated multimedia system. However, as previously described, it does not meet the TRIM design goals for a flexible architecture.

In general, none of the current models is a sufficiently coupled multimedia model that accounts for inherent “feedback” loops or secondary emissions (i.e., re-emission of deposited pollutants) or releases to specific media, or that provides the temporal and spatial resolution critical in estimating exposures. While it is unknown as to the degree to which modeled results would differ between current models and a truly coupled multimedia model, models that are not truly coupled have been considered to lack scientific credibility. Therefore, OAQPS determined it was necessary to undertake efforts to develop a truly coupled multimedia model.

3.3 Uniqueness of TRIM.FaTE

Among the unique features of TRIM.FaTE are: (1) its flexibility to be formulated at different spatial and temporal scales, (2) the ongoing development of an algorithm library, and (3) a full accounting of all of the chemical mass that enters and leaves the environmental system.

TRIM.FaTE was developed to meet OAQPS modeling needs (Section 1.3) and fit the TRIM design criteria (Section 2.2). To meet these goals requires a multimedia framework. Also

required are true coupling of multiple media during a simulation (similar to Mackay-type models) and a level of spatial and time-series resolution to date only obtained from linked single-media numerical simulation models. The TRIM development team determined that TRIM must: (1) address varying time steps (of one hour or greater) and provide sufficient spatial detail at varying scales (site-specific to urban scale); (2) provide true "mass-conserving" results; (3) have the transparency needed for use in a regulatory context; and, (4) be a truly coupled multimedia model rather than a set of linked single media models. After reviewing currently available multimedia models, the team determined that none of the available models offered all of these features. As a result, the team engendered a new model framework that is distinct from other multimedia models and unique among the current arsenal of EPA models.

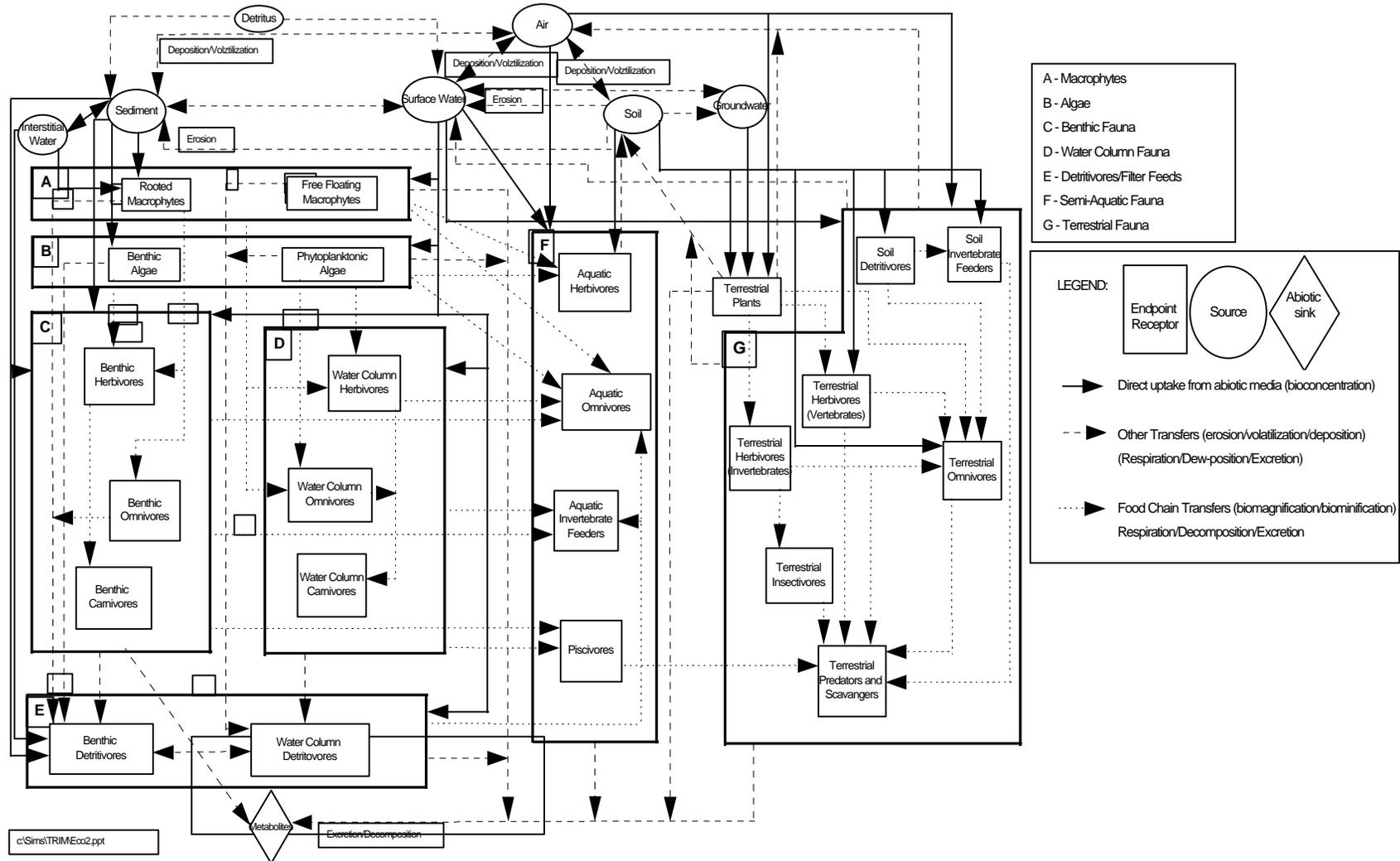
TRIM.FaTE has a mathematical approach (Section 3.4), which makes possible: (1) different mixes of compartment numbers, types, and links; (2) a unified approach to mass transfer based on an algorithm library, which allows the user to change mass transfer relationships among compartments without creating a new program; and, (3) the flexibility to match a simulation to the spatial and temporal scales needed for a broad range of pollutants and geographical areas. Although some applications of TRIM.FaTE may resemble a simple fugacity-based compartmental model, it can be scaled to simulate time-series and spatial resolutions that current regional fugacity-type models could not handle. The mathematical linking in TRIM.FaTE enables it to simulate mass distribution within a system and attain a degree of precision not yet achieved by other models.

3.4 TRIM.FaTE Basic Concepts and Terminology

The development of TRIM.FaTE began with a "conceptual blueprint" of the relationships and processes that describe chemical transport within an ecosystem. This blueprint is shown in Figure 3-1. On this figure, the biota are represented by squares, biotic sinks are represented by diamonds, and the abiotic media are represented by ovals. The various lines show possible chemical transfers occurring between each of the components of the ecosystem. Any environment can be thought of as a complex system, and thus can be represented using systems models that follow from the principles of systems theory. Lines may represent transfers of energy or matter, and in this case, the transfers represent chemical contaminants. All of the different locations, geographical features, and ecosystems are then subsystems interacting with each other.

Because the terminology used in the world of multimedia modeling can have multiple meanings and implications, it is critical in the conceptualization of any complex model that terminology used be defined specifically within the framework of that model. Multimedia models by nature are multidisciplinary. Terminology can be confusing because a single term will have dramati-

Figure 3-1
Conceptual Blueprint for TRIM.FaTE



cally different meanings in different disciplines. To avoid confusion, discussion of TRIM.FaTE terminology is presented in this section. Following the description of the terminology, a summary is provided of the mathematical basis for TRIM.FaTE. In addition, a glossary is included in Appendix A.

In the TRIM.FaTE model, the transport of multiple pollutant species in an ecosystem is set up as a mass exchange among a set of systems used to represent spatial locations, collections of environmental phases, and chemical species. The primary features of interest are the chemical inventory and the chemical concentrations of the system as a function of time in the various components of the modeled system. These values are called **state variables** since they describe the state of the system while it is varying³⁴.

The system being modeled is assumed to be partitioned into regions of three-dimensional space. Each such region is referred to here as a **volume element**. Typically, only one type of abiotic medium is contained in a volume element. This term is introduced as a matter of convenience for organizing objects that have a natural spatial relationship. The region represented by a volume element could be a cube or more complicated shape. A volume element usually shares a surface with other volume elements. The spatial resolution of volume elements may vary from application to application, and even within a single application.

Contained within volume elements are **domains**. The term “domain” is a loose equivalent of what is referred to as “media” in environmental fate and transport modeling literature. However, the term “media” was considered to be limited in its scope because it generally brings up images of abiotic systems such as soil or air, while TRIM.FaTE includes both abiotic and biotic systems. Therefore, the term domain was adopted for TRIM from the principles of systems theory to allow for more flexibility in its definition. A **domain** is the material that contains a chemical(s). It is currently assumed that, within any domain, a chemical is uniformly distributed throughout the volume occupied by that domain. In addition, the various phases (gases, liquids, solids) that make up a domain are assumed to be in equilibrium with respect to chemical partitioning. Domains can be thought of in both a general and specific sense within the TRIM.FaTE modeling structure. In a general sense, a **domain type** is defined to classify overall system components such as soil, water, or mouse, or more specific components such as surface soil or vadose zone soil. A specific manifestation of a domain type is a **domain instance**. Domain instances belong to the same domain type with similar attributes. One domain instance is distinguished from another by the values that define its composition attributes at a given location. For example, any “soil” domain

type consists of gas, liquid, and organic- and mineral-solid phases. As a domain instance, a surface-soil domain instance typically has more organic carbon than a vadose-soil domain instance. Moreover, a vadose-soil domain instance will typically have a higher water-volume fraction than a root-soil domain instance. Two different mouse domain instances may differ by the population size attribute. There can be multiple domain instances within a volume element, i.e., a worm domain instance may exist simultaneously with a surface soil domain instance in a volume element. Typically, one abiotic domain type (soil, water, air), but multiple biotic domain types (worm, plants), can exist within a volume element. When there is no need for additional clarification between domain types and domain instances, these will be referred as domains in TRIM.FaTE literature.

The set of all domain instances is assumed to contain all of the chemical mass within the ecosystem, excluding **sources**. A source is an external component that transfers chemical mass directly into the domain instances. Examples of sources would include the factory emissions of a chemical into an air domain, or the influx of chemical in a river from outside the modeled system.

Associated with each domain instance is an **inventory address or cell**. A cell is a bin within the computer code, and these cells collectively account for all potential locations of mass within the ecosystem, and the pollutant sources and sinks outside the ecosystem that are required to balance the overall mass flow. Each **cell** is uniquely defined by three indices. The first index is the volume element. The second index identifies the domain containing the chemical at a given location. The third index is the chemical species.

An important aspect that is tracked for each cell is the list of other cells in the system with which it potentially exchanges chemical mass. It is necessary only to store in this list the cells from which the cell receives mass. Elements of this list are referred to as **links**. With each link is associated a **sending cell** and **receiving cell**. The sending cell is the cell from which the chemical is potentially transported, and the receiving cell is the cell that receives the chemical. Each specific link for any chemical may have unique properties, and hence must be considered as an object separate from all other links. For example, a link between two particular soil cells may contain information on the advective flow from the sending cell to the receiving cell. Another example is the worm-to-soil cell link, which contains information on the ingestion rate of soil by worms.

The link between domains includes information on the potential exchange of chemical between the two domains. This information includes a **transfer factor**, which is the instantaneous flux from the sending domain to the receiving domain per unit chemical mass in the sending domain.

Transfer factors are calculated based on transport and fate processes such as advection, diffusion, dispersion, reaction, and bioaccumulation. The mathematical basis for these transfer factors is discussed in Section 3.4. The transfer factor is determined by use of the methods in a central repository of algorithms, called an **algorithm library**. Algorithms in TRIM.FaTE are equations that express the transfer factor as a function of a set of variables. This function is specific to the locations, domains, and chemical species represented by the linked cells.

It is stressed that the algorithm library is not intended to consist of only documented methods; instead, the methods must be properly entered in some standard manner so that they can be accessed by other software. For first-order transfers, methods have been developed for converting typically encountered concentration-based equations to mass balance form. Appendix B presents generalizations for algorithm development. All major methods of pollutant movement in the environment are frequently modeled with first-order methods. These include advective processes, diffusive processes, and bioaccumulation.

3.5 Governing Mass Balance Equations

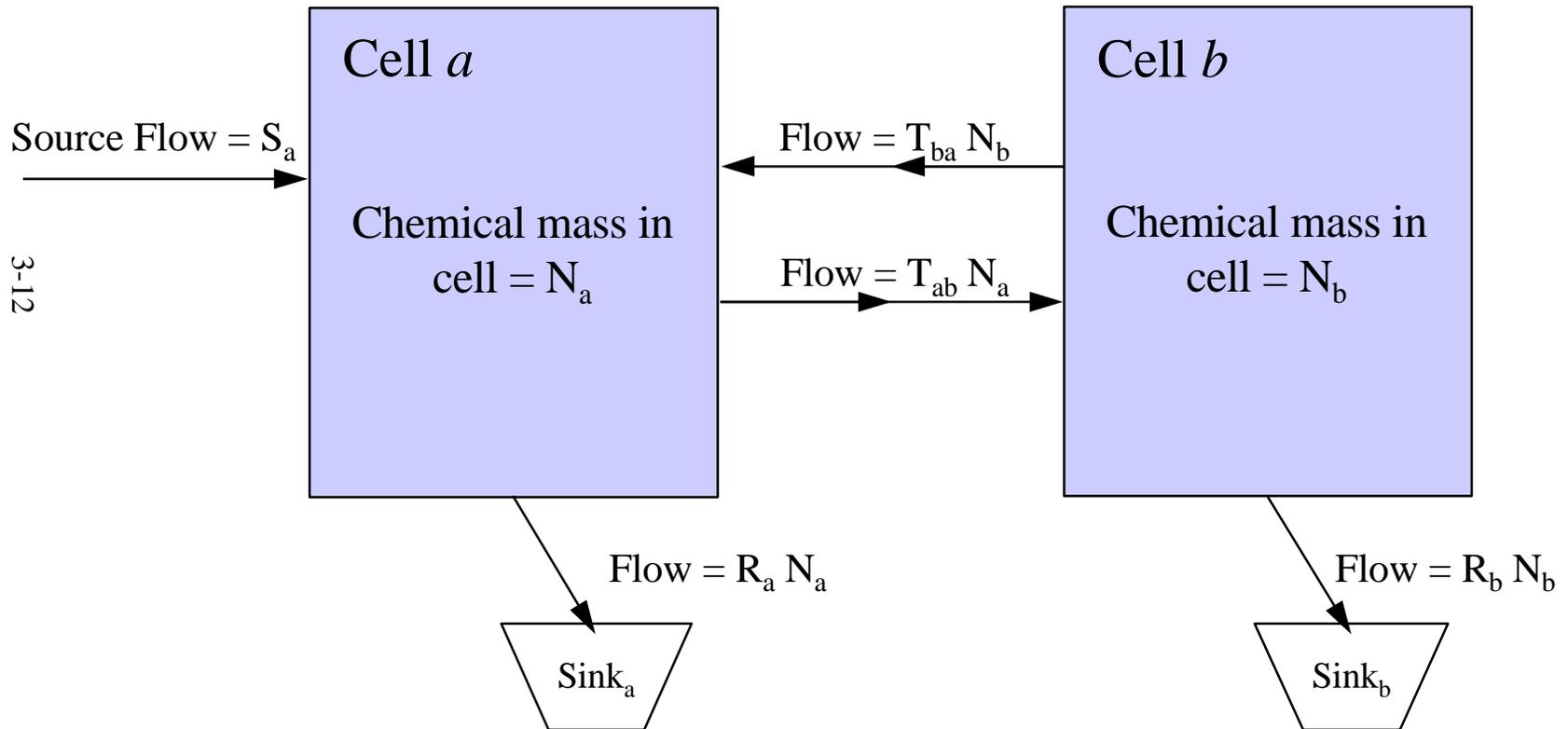
The TRIM.FaTE model is being developed with an emphasis on conserving chemical mass. This means that the entire quantity of the chemical is tracked throughout the system being modeled. When applied to a specific domain (e.g., soil or a mouse population), this implies that, over a given time period, the amount of the chemical in the domain at the end of the period is equal to the amount of the chemical in the domain at the beginning of the period, plus the gains of the chemical that occurred during the time period, minus the chemical that was lost from the domain during the time period.

Currently, the mass balance approach has been implemented primarily for first-order linear processes. Therefore, the discussion here is limited to models of this type. It is important to note that higher order non-linear methods can also be implemented within this structure.

A simplification of a transfer process is shown in Figure 3-2 for a system of two cells, where it is assumed that the fluxes of chemical mass are first-order processes. Denoting by $N_a(t)$ and $N_b(t)$ the mass of chemical in cells a and b , respectively (in units of *mass*), it can be seen that:

Figure 3-2

Example of First Order Transfer Process for Two Cells



$$\begin{aligned} \text{Gains for cell } a &= S_a + T_{ba}N_b \\ \text{Losses for cell } a &= T_{ab}N_a + R_aN_a \end{aligned}$$

and

$$\begin{aligned} \text{Gains for cell } b &= T_{ab}N_a \\ \text{Losses for cell } b &= T_{ba}N_b + R_bN_b \end{aligned}$$

where:

- S_a = chemical source in cell *a*, units of *mass/time*
- T_{ab} = transfer factor for movement of chemical from cell *a* to cell *b* during time interval, units of */time*
- T_{ba} = transfer factor for movement of chemical from cell *a* to cell *b*, units of */time*
- R_a = reaction loss of chemical in cell *a*, units of */time*
- R_b = reaction loss of chemical in cell *b*, units of */time*.

The constraint that mass balance must be preserved means that, over any time interval, the change in mass in a cell is equal to the gains minus the losses in mass over the time interval. The instantaneous change in mass with respect to time is the derivative with respect to time, denoted by dN_a/dt . Thus, the mass balance constraint, when applied to the simple system discussed here, yields a system of two linked differential equations:

$$\begin{aligned} \frac{dN_a}{dt} &= S_a + T_{ba}N_b - (R_a + T_{ab})N_a \\ \frac{dN_b}{dt} &= T_{ab}N_a - (R_b + T_{ba})N_b \end{aligned}$$

Additional terms are needed to properly account for the chemical mass. In particular, the fate of the chemicals after reacting must be tracked. For this reason, two additional cells are added to the system, and serve as the repository of the chemicals after reaction. These are referred to as “sinks,” since once the chemical is transferred into these cells, it no longer moves to any other cells. While clearly the chemical would continue to move in its altered form throughout the

system, for this example, this history is not of interest. Denoting by $Sink_a$ and $Sink_b$, the mass in the reaction sinks for cells a and b , respectively, the complete system is:

$$\begin{aligned}\frac{dN_a}{dt} &= S_a + T_{ba}N_b - (R_a + T_{ab})N_a \\ \frac{dN_b}{dt} &= T_{ab}N_a - (R_b + T_{ba})N_b \\ \frac{dSink_a}{dt} &= R_aN_a \\ \frac{dSink_b}{dt} &= R_bN_b\end{aligned}$$

or, in matrix form:

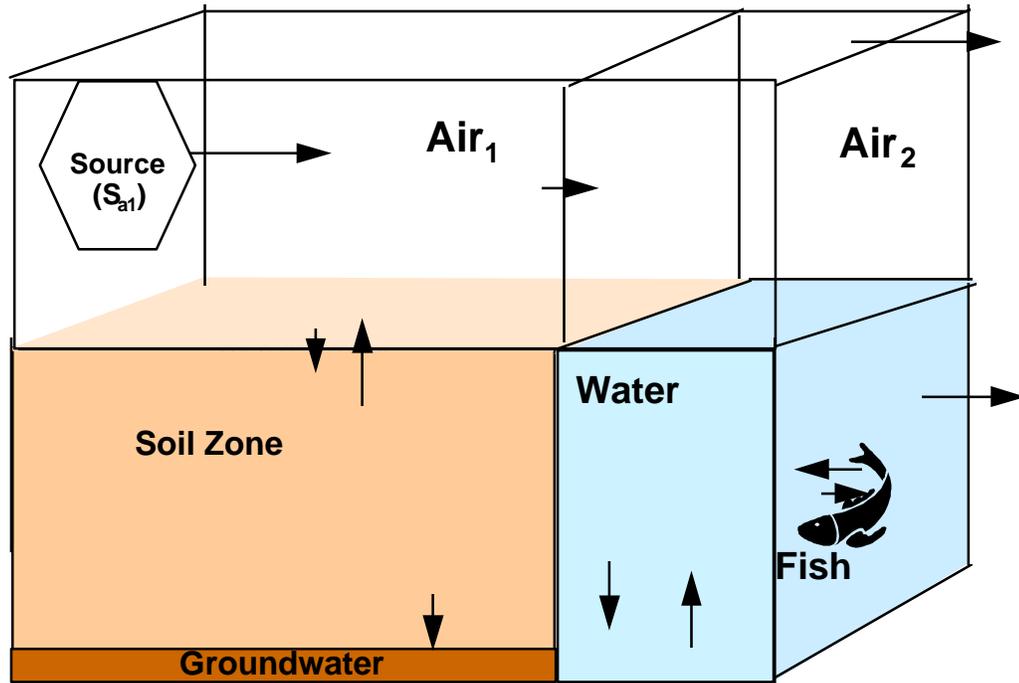
$$\begin{bmatrix} dN_a/dt \\ dN_b/dt \\ dSink_a/dt \\ dSink_b/dt \end{bmatrix} = \begin{bmatrix} -(T_{ab}+R_a) & T_{ba} & 0 & 0 \\ T_{ab} & -(T_{ba}+R_b) & 0 & 0 \\ R_a & 0 & 0 & 0 \\ 0 & R_b & 0 & 0 \end{bmatrix} \begin{bmatrix} N_a \\ N_b \\ Sink_a \\ Sink_b \end{bmatrix} + \begin{bmatrix} S_a \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Application of this methodology to a simplified ecosystem with ten cells, as shown in Figure 3-3, yields a transition matrix equation of the form:

$$\frac{d}{dt} \begin{bmatrix} N_{a1} \\ N_{a2} \\ N_s \\ N_w \\ N_f \\ N_g \\ N_{Ra} \\ N_{Rw} \\ N_{Rs} \\ N_{Rf} \end{bmatrix} = \begin{bmatrix} -K_{a1} & 0 & T_{sa1} & T_{wa1} & 0 & 0 & 0 & 0 & 0 & 0 \\ T_{a1a2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ T_{a1s} & 0 & -K_s & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ T_{a1w} & 0 & T_{sw} & -K_w & T_{fw} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & T_{wf} & -K_f & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & T_{sg} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ R_a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & R_w & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & R_s & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & R_f & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} N_{a1} \\ N_{a2} \\ N_s \\ N_w \\ N_f \\ N_g \\ N_{Ra} \\ N_{Rw} \\ N_{Rs} \\ N_{Rf} \end{bmatrix} + \begin{bmatrix} S_{a1} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Figure 3-3

Simplified Ecosystem



The ecosystem consists of:

- Two Air Cells
- Soil Cell
- Groundwater Cell (sink)
- Surface Water Cell
- Fish Cell
- Four sinks

TOTAL = 10 Cells

where:

$$\begin{aligned}
 S_{a1} &= \text{source term for air Cell 1} \\
 T_{ij} &= \text{transfer factors for Cell I to j} \\
 N_i &= \text{mass of pollutant in Cell i} \\
 K_{a1} &= R_{a1} + T_{a1w} + T_{a1s} + T_{a1a2} \\
 K_s &= R_s + T_{sw} + T_{sa1} + T_{s0} \\
 K_f &= R_f + T_{fw} + T_{f0} \\
 K_w &= R_w + T_{ws} + T_{wa} + T_{wf} + T_{w0}
 \end{aligned}$$

Applying this same approach to a general system with M cells (including all sinks), and allowing the transfer factors and source terms to depend on time as well, results in a system of linked differential equations of the form:

$$d\mathbf{N}/dt = \mathbf{A}(t)\mathbf{N} + \mathbf{s}(t), \mathbf{N}(t_0) = \mathbf{N}_0$$

where:

$$\begin{aligned}
 \mathbf{N}(t) &= \text{an } M\text{-dimensional vector whose } i\text{th entry is the mass in the } i\text{th cell} \\
 \mathbf{A}(t) &= \text{an } M \times M \text{ time-dependent matrix} \\
 \mathbf{s}(t) &= \text{an } M\text{-dimensional vector accounting for the source terms in each cell.}
 \end{aligned}$$

The matrix $\mathbf{A}(t)$ is referred to as the *transition matrix* for the system. This term is borrowed from Markov theory, although the model is not strictly a Markov process. The vector \mathbf{s} accounts for pollutant sources located within specific cells. The vector \mathbf{N}_0 is the initial distribution of mass among the cells.

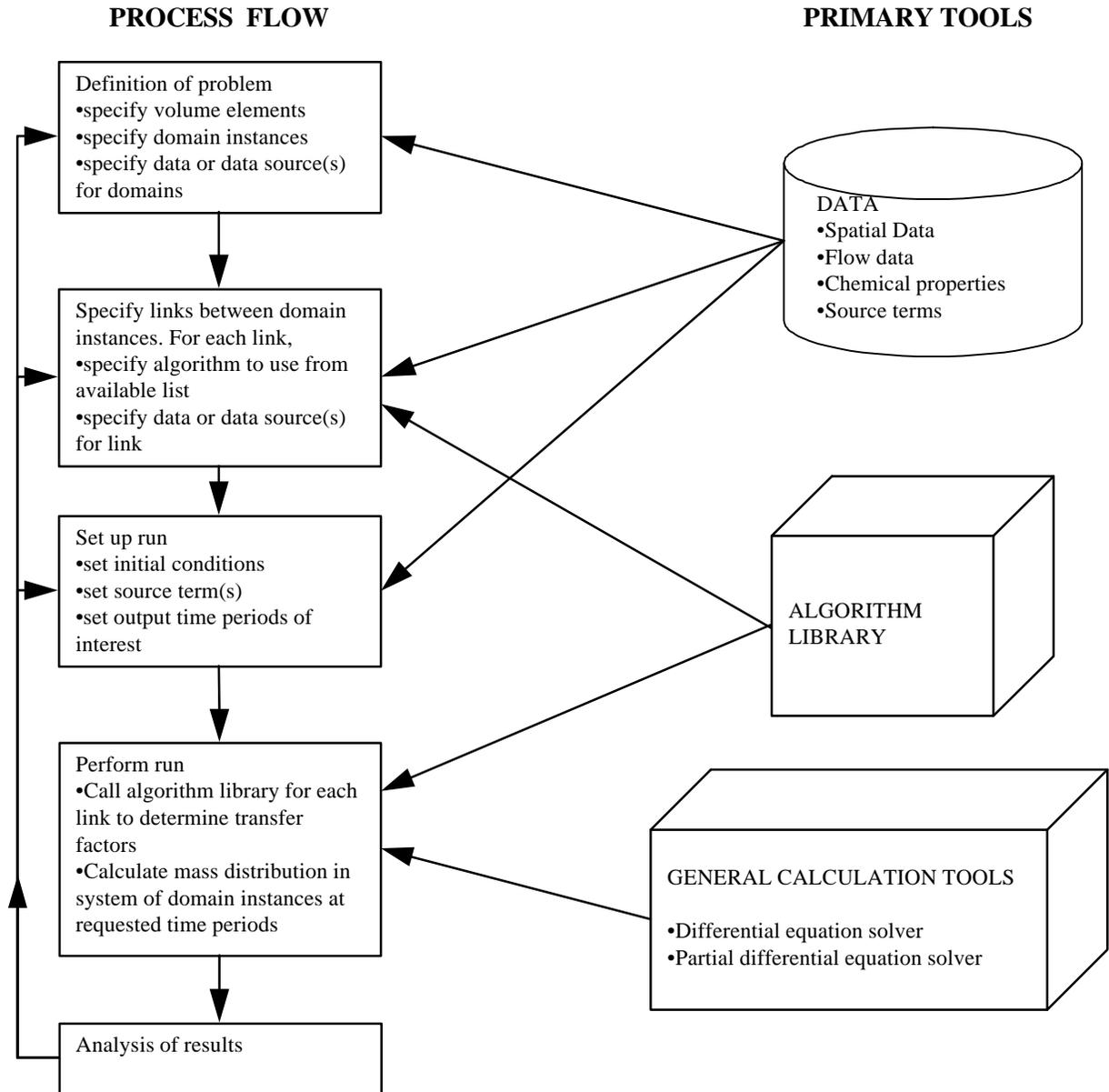
3.6 Modeling Approach

This section summarizes the general features of the application of the conceptual approach previously described.

One of the primary features of the application of the TRIM approach is that it is to be an iterative and flexible process. When the modeling process is first started, there is a general sequence that must be followed. After the initial step, however, there is no fixed order in which the modeling steps are necessarily performed. This process is shown in Figure 3-4. The boxes on the left side of the figure represent a partitioning of the modeling sequence into five broad areas. These areas include: basic problem definition, specification of links, setting up a run, performing a run, and analysis of results. The particular division into five such areas is somewhat arbitrary, and in an actual application, it may be that the progression is not quite as linear as that shown in the figure.

Figure 3-4

Structure of TRIM.FaTE



However, all of these steps are necessary. The vertical arrows between these boxes represent the possible order of events in the modeling process. The arrows on the left side of the boxes indicate the iteration that may be necessary or desired.

The shapes under the heading “Primary Tools” represent the primary tools used in the modeling process. The arrows from these shapes to the flow boxes indicate where in the modeling process these tools would be used. To focus on key aspects of the TRIM.FaTE approach, only selected tools are shown. There are other tools that may be necessary that are not included in this figure. Such tools would include pre/postprocessing software that may automate some aspects of the process, and general user interface software.

3.6.1 Problem Definition

The first step requires the general problem definition. During this step, the chemical(s) to be modeled and the initial spatial features of the ecosystem are determined. In the nomenclature previously discussed, the volume elements and domain instances within the volume elements are specified. For the first cycle through the simulation process, the spatial scales may be crude and the number of domain instances may be small. It will be necessary at this step to specify various types of data, or simply the sources of the data (e.g., a remote database). Data types include spatial information about the ecosystem, chemical-specific environmental data (e.g., degradation rates in various domain types), and data for the specified domain instances (e.g., soil densities and organic carbon content for soil domains).

3.6.2 Link Setup

The second step shown in Figure 3-4 specifies the links between the domain instances. Two domains are considered “linked” if there is a direct means by which the chemical can be exchanged. This definition does not include “indirect” links that result from a chain of direct links (e.g., chemical is transported in eroding soil to a water domain, and subsequently taken up by a fish population). The system of links is one of the most critical components of the model. By specifying a link between two domains, it is assumed that some method exists by which to estimate the transfer of chemical through the link. If this method is already included in the algorithm library, then it is only necessary to specify the data (or data source) for this link and which algorithm to use. These data may depend on both of the domains in the link (e.g., erosion flow rate for link between a soil domain and a water domain). These data do not include information about the mass of the chemical, as tracking the inventory of chemical mass with time is the purpose of the model. If the algorithm is not in the algorithm library, then it must be “added” so that it can be accessed by the underlying software.

3.6.3 Simulation Setup

The third step shown in Figure 3-4 is the preparation of a simulation after the volume elements, domain instances, and links have been specified. This involves specifying the initial distribution of chemical mass in the domains, specifying any source terms considered within domains, and specifying the output time period(s) of interest. The initial conditions may be specified as concentrations, which are then converted to mass form for the model. The “DATA” drum is connected to this step because data are necessary for the initial conditions and source term(s). The initial conditions and source terms may be estimated from monitoring data available, or from the results of another model.

3.6.4 Simulation Implementation

The fourth step is the actual running of the model, where the movement of the chemical(s) through the domains is simulated for the specified time period(s). The exact manner in which this is performed depends on the algorithms chosen. For each link between domains, a call is made to the algorithm library to determine the transfer factors that indicate the potential exchange of chemical mass. If all algorithms involve only first-order processes, then movement of the chemical will be simulated with a system of linked differential equations, the solution of which would be found using a differential equation solver. For more complicated algorithms, other tools would be necessary (e.g., a method of solving partial differential equations).

3.6.5 Result Analysis

The last step shown in Figure 3-4 is the analysis of the results generated for the modeled system. These results include the time history of the chemical mass and associated concentrations in the domains. This step would also include postprocessing analysis of the results and use of the results in other parts of the TRIM.

3.7 Sensitivity Analysis

An important aspect of the TRIM is the integration of sensitivity and uncertainty analyses methods into the model framework. The reasons for a sensitivity analyses are to identify important inputs with respect to outcome variance in order to direct efforts related to:

- Additional data collection
- Additional research
- Stratification of the population.

Many of the parameters used in modeling of natural systems are uncertain or variable. It is critical to confront sources and ranges of parameter variance for several reasons. Among them are the need to determine the range of possible outcomes of the model, and the need to determine what parameters are the important contributors to the range of outcome values generated by the model.

The TRIM framework is designed to provide for a tiered uncertainty/sensitivity analyses in several ways. All inputs to TRIM are entered in parameter tables where value distributions are the default option and the labels “uncertain” or “variable” can be applied to make initial classifications. The capability to conduct a joint uncertainty and variability analysis is a goal of TRIM. Currently, the capability exists to conduct simple sensitivity analyses. Ultimately, Monte Carlo assessments and uncertainty importance assessment capabilities will be an integral part of TRIM.FaTE. Some limited assessment of model uncertainty is provided through the option of selecting from alternate transport/transformation algorithms from an algorithm library.

3.8 Example Calculation of Transfer Factors

In previous sections, the term “transfer factor” is used to describe the potential transfer of chemical mass between two domain instances. This section shows an example of how these transfer factors are determined for a first-order process, starting with a model for estimating the concentration of a chemical in fish.

Thomann³⁵ gives the following model for calculating the concentration in fish:

$$\frac{dC_f}{dt} = k_u \times C_{WD} + K_D \times \sum P_i \times C_{D,i} - (k_E + k_{eg} + R_M + K_G) \times C_f$$

where:

- C_f = concentration in fish (micrograms per kilogram [$\mu\text{g}/\text{kg}$])
- k_u = uptake rate from water via the gills (1/kg-day)
- C_{WD} = dissolved chemical concentration in water (micrograms per liter [$\mu\text{g}/\text{L}$])
- k_D = chemical uptake from food (kg food/kg fish/day)
- P_i = proportion of the diet consisting of food item I
- $C_{D,i}$ = chemical concentration in food item I ($\mu\text{g}/\text{kg}$)

- k_E = elimination via fecal egestion (1/day)
- k_{eg} = elimination via the gills (1/day)
- R_M = metabolic transformation of chemical (1/day)
- k_G = dilution contaminate concentration from growth (1/day).

This algorithm was derived to estimate concentrations in individual fish of a species. Initially, the model is generalized for a population of two fish, and then for the case of an arbitrary number of fish. The previous equation is further simplified by assuming that there is no uptake through other food items. Also, the elimination via fecal egestion and the metabolic transformation factors are neglected. Thus, for two fish with concentrations C_{f1} and C_{f2} the previous equation can be rewritten as:

$$\frac{dC_{f1}}{dt} = k_{u1} \times C_{WD} - k_{eg1} \times C_{f1}$$

$$\frac{dC_{f2}}{dt} = k_{u2} \times C_{WD} - k_{eg2} \times C_{f2}$$

To convert the concentrations to masses it is assumed that:

$$C_{WD} = \frac{N_w}{V_w},$$

$$C_{f1} = \frac{N_1}{m_1},$$

$$C_{f2} = \frac{N_2}{m_2}$$

where:

- m_1 = mass of fish 1 (kg)
- m_2 = mass of fish 2 (kg)
- N_1 = mass of contaminant in fish 1 (μg)
- N_2 = mass of contaminant in fish 2 (μg)
- V_w = volume of surface water cell (L).

Substituting results in:

$$\frac{d(N_1/m_1)}{dt} = k_{u1} \frac{N_w}{V_w} - k_{eg1} \frac{N_1}{m_1}$$

$$\frac{d(N_2/m_2)}{dt} = k_{u2} \frac{N_w}{V_w} - k_{eg2} \frac{N_2}{m_2}$$

Adding these equations yields the mass transfer equations for the total fish population consisting of the two fish, as follows:

$$\frac{d (N_1/m_1 + N_2/m_2)}{dt} = (k_{u2} + k_{u1}) \frac{N_w}{V_w} - (k_{eg1} \frac{N_1}{m_1} + k_{eg2} \frac{N_2}{m_2})$$

Making the simplifying assumptions that individual fish mass is represented by a population average m_f ($m_1=m_2=m_f$), and that $k_{u1}=k_{u2}=k_u$ and $k_{eg1}=k_{eg2}=k_{eg}$, yields:

$$\frac{d \left(\frac{N_1+N_2}{m_f} \right)}{dt} = 2 k_u \frac{N_w}{V_w} - k_{eg} \frac{N_1 + N_2}{m_f}$$

This equation can be generalized from two to n_f fish, with $N_f (= N_1+N_2)$ being the total pollutant mass in the fish domain to yield the following generalized mass transfer equation for a fish domain:

$$\frac{dN_f}{dt} = n_f k_u m_f \frac{N_w}{V_w} - k_{eg} N_f$$

Implicit in the previous equation is the assumption that the mass of an individual fish is constant over the time of the simulation. It may be noted that the dilution due to growth factor (k_G) is not

included in this equation because k_G is based on concentrations not mass. Transfer factors for the fish domain are now given by:

$$T_{wf} = \frac{n_f k_u m_f}{V_w}$$

$$T_{fw} = k_{eg}$$

where:

T_{wf} = transfer factor for exchange of chemical mass from water to fish population (/day)

T_{fw} = transfer factor for exchange of chemical mass from fish population to water (/day).

3.9 Summary of TRIM.FaTE Approach

In this chapter, the TRIM.FaTE framework has been introduced by describing a unified conceptual approach to multimedia mass-balance models. The term "unified" refers to the fact that one approach has been generalized to all components of a multimedia environment, including ecosystem components. The mass-balance approach for first-order systems reduces to a set of linear ordinary differential equations was illustrated. However, the approach is not limited to first-order linear methods. The modeling approach provides a flexible, iterative process of simulating the movement of chemicals in a multimedia environment. This makes the approach useful for addressing different types and aquatic and terrestrial ecosystems and also for human exposure assessment. It is important to note that the approach used is not based on linking different models for different compartments or domain instances. Instead, the entire system is represented in a single informational structure, i.e., a large matrix. In the next chapter, more specific examples are presented of the multimedia models that can be constructed using this type of flexible and iterative process.

4.0 TRIM.FaTE Prototype Development

This chapter provides a description of the process of applying the TRIM.FaTE methodology (Chapter 3.0) to cases of increasing complexity (referred to as “prototypes”). Section 4.1 discusses the implementation of the prototypes; Section 4.2 describes the development process for each prototype; Section 4.3 addresses the features of the prototypes, including the types of domains and links simulated; and Section 4.4 discusses the processes used to simulate links. The goal of this chapter is to illustrate the flexibility of TRIM.FaTE for application at different levels of spatial and temporal resolution. This chapter also serves to illustrate how different multimedia configurations with TRIM.FaTE are set up.

4.1 Implementation of Prototypes

The concepts discussed in the previous chapter have been implemented using a combination of Visual Basic, Fortran, and Microsoft Excel™ software. These implementations are documented in detail in the technical support document¹.

An object-oriented architecture, similar to that shown in Figure 3-2, was implemented using Visual Basic 5 imbedded within Excel 97 to model the hierarchy of components of TRIM.FaTE. This hierarchy includes volume elements, domain types, domain instances in the volume elements, and links between the domains. The coding architecture is not tied to any specific ecosystem configuration. A preliminary algorithm library that utilizes this coding architecture was also implemented.

If all transport processes are simulated as first-order process, this results in a system of linear ordinary differential equations. This system must be solved to determine the redistribution of chemical mass as a function of time. For TRIM.FaTE, this system is solved using the Livermore Solver for Ordinary Differential Equations (LSODE)³⁶, a Fortran program freely available via several online numerical algorithm repositories.

The LSODE subroutine solves systems of first order ordinary differential equations of the form³⁷:

$$dy/dt = F(t,y), y(t_0) = y_0$$

where y is an n -dimensional time-dependent vector, i.e.,

$$y(t) = [y_1(t), y_2(t), \dots, y_n(t)].$$

The system of differential equations can be stiff or non-stiff. In the stiff case, it treats the Jacobian matrix as either a full or banded matrix. It uses Adams methods (predictor-corrector) in the non-stiff case, and backward differentiation formula methods in the stiff case. The linear systems that arise are solved by direct methods (LU factorizations). LSODE supersedes the older GEAR and GEARB packages.

The only restriction on the size of the system of differential equations is that imposed by computer memory. This code was modified so that it could be accessed by Visual Basic 5 in Excel 97. Another Fortran code was used, in a similar manner, to determine the steady state solution to the system of linear differential equations³⁸.

Microsoft Excel spreadsheets were used for general preprocessing, postprocessing, and data storage (additional databases for spatial data were also created using Visual Basic and accessed by Excel). Excel spreadsheets also served as a convenient interface to the Visual Basic and Fortran subroutines.

The approach taken for testing the methodology made it possible to investigate the implications of draft algorithms and to work on the development of a flexible system for addressing conceptual site models with many domains. The pre- and postprocessing for the ultimate implementation of TRIM.FaTE may require a more sophisticated platform. However, with some modification, much of the Visual Basic code, and all of the Fortran code, can be used in other computer programming languages.

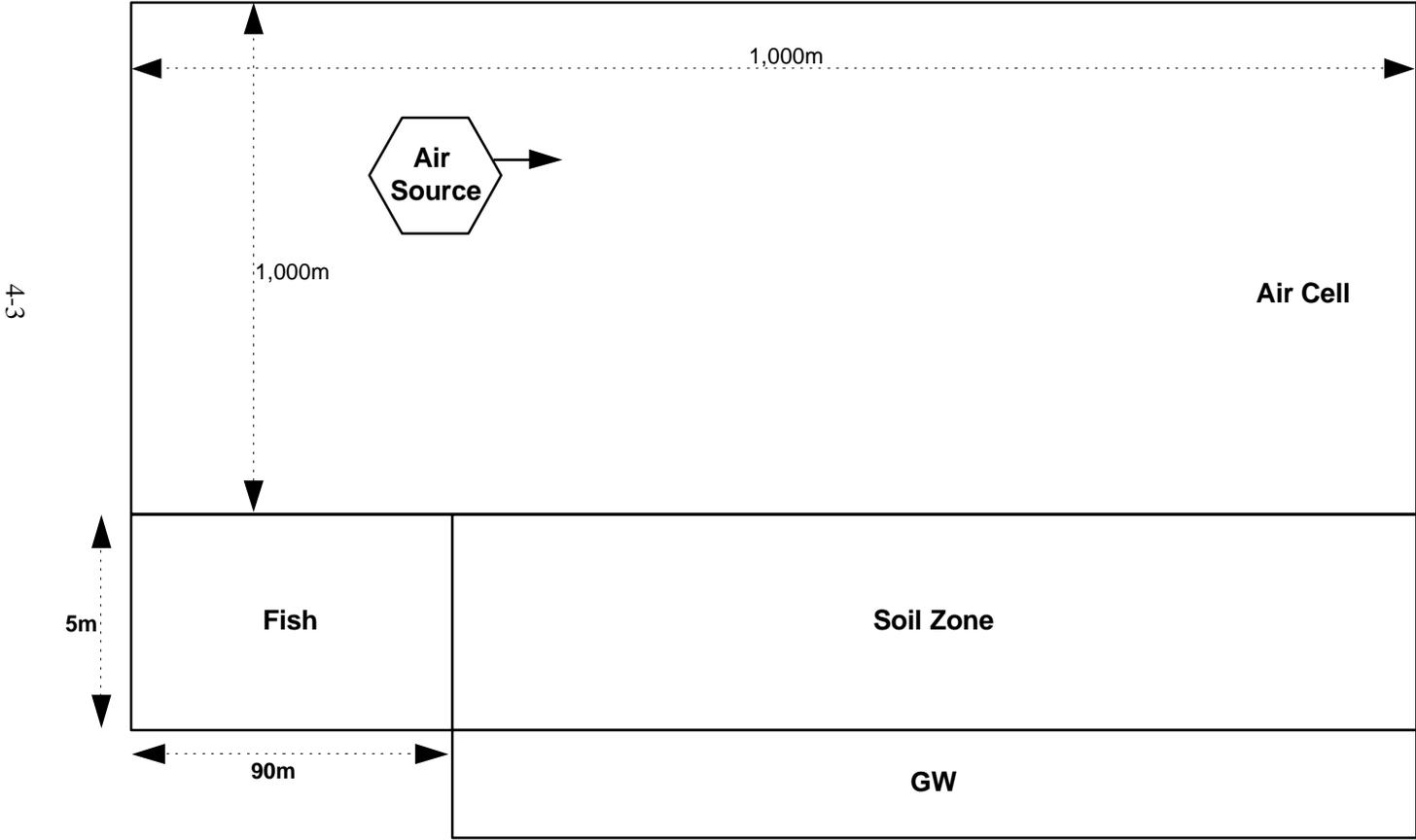
4.2 Prototype Development

Multiple prototypes were developed with increasing complexity to model the movement of a pollutant through an ecosystem. This section describes features of the prototypes in increasing order of complexity.

4.2.1 Prototype 1

Prototype 1 (P1) was set up to test the mass transfer methodology (Chapter 3.0) and the LSODE utility. Air, soil, groundwater, surface water, and fish domains were simulated in P1 as seen in the conceptual site model shown in Figure 4-1. P1 includes a uniform volume source emission of benzene into the air volume. Benzene was selected because most of its transfer factors were readily available from CalTOX³⁹.

Figure 4-1
Conceptual Site Model for Prototype 1



Some transfer factors were derived independently of CalTOX for the air to air sink, soil to groundwater, fish to water, and water to fish transfers. The remaining factors were taken directly from CalTOX. The dimensions of the terrain were adapted from CalTOX to facilitate comparison of results. Chemical reaction was not simulated in this prototype.

The runs produced estimates of benzene mass throughout the system, and no problems were experienced in running the LSODE subroutine. The resulting mass distribution of benzene in various domains was commensurate with theoretical expectations and showed that TRIM.FaTE is relatively easy to implement for a simple ecosystem. These results prompted further testing of the modeling approach on a more complex ecosystem.

4.2.2 Prototype 2

Prototype 2 (P2) includes a more spatial detail than P1 and more sophistication than P1 in both the types and number of domains used. Unlike P1, P2 included multiple volume elements for both the soil and air domain types and included the use of plant and sediment domains. In addition, the links between cells had multiple-phase (i.e., gas, liquid, and solid) mass transfers. P2 included a volume source emission of benzo(a)pyrene (B[a]P) into only one of the air volumes. This made possible a very simple representation of spatial transport. B(a)P was selected as a test chemical for this and subsequent prototypes because of its persistence in the environment and the fact that it is a pollutant of interest to EPA's Risk and Exposure Analysis Group. The derivation of the transfer factors are described in detail in the technical support document¹. The conceptual site model for P2 is shown in Figure 4-2.

Multiple-phase (liquid, gas and solid) transport within a domain was introduced in P2. The phases are assumed to be at chemical equilibrium, with the ratios of the concentrations in the individual phases constant.

4.2.3 Prototype 3

The Prototype 3 (P3) code and input data are significantly more complex than either P1 or P2. P3 was developed both to incorporate lessons learned from P2, which has a refined set of abiotic algorithms, and to set up the TRIM.FaTE model for the case study model run Prototype 4 (P4). P3 includes a conceptual site that dimensionally represents the ecosystem of the test area for P4. The conceptual site model for P3 is shown in Figure 4-3. The vertical dimensions of individual air cells are not indicated because these dimensions were allowed to vary with time according to

Figure 4-2
Conceptual Site Model for Prototype 2

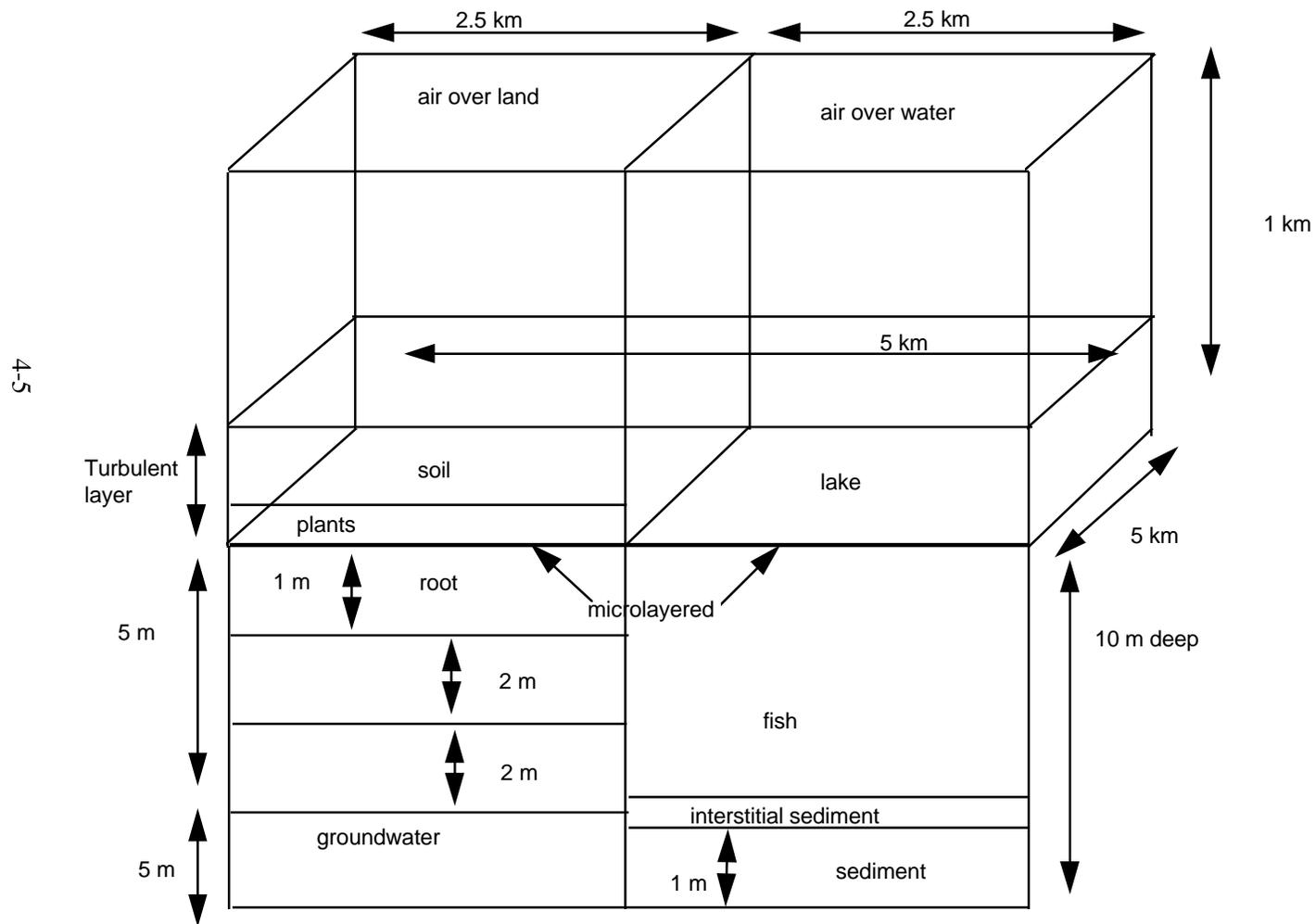
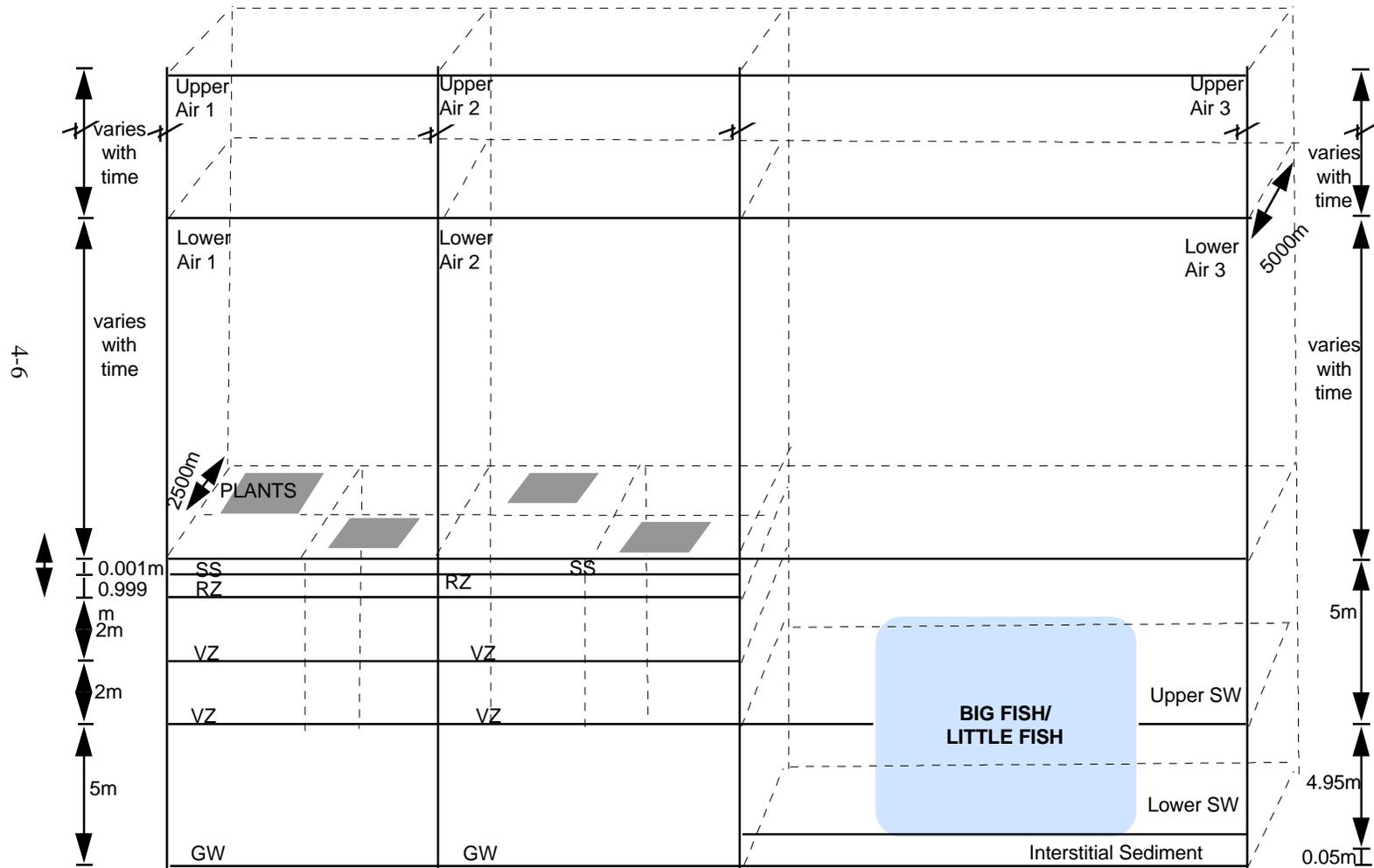


Figure 4-3
Conceptual Site Model for Prototype 3



a set of specified meteorological conditions. The soil and surface water domains were split into finer grid structures relative to P2, and several new biotic algorithms were added. The source term simulated in P3 was a volume-source emission of B(a)P into only one of the four air volume elements. This was used to make an approximation to a continuous point-source release.

The differences of P3 relative to P2 include:

- Addition of terrestrial earthworms, kingfisher, and mouse domains
- Addition of aquatic food-web system
- Addition of cells with varying heights for the air domain to increase complexity
- Division of soil cells horizontally to add complexity to soil domain
- Introduction of “thermoclines” and refinement of mixing for surface water
- Refinement of plant domain algorithms
- Refinement of soil diffusion algorithms
- Addition of erosion in the soil domain
- Refinement of groundwater algorithm
- Introduction of flexible code design
- Introduction of temporal variation for a few key input parameters.

4.2.4 Prototype 4

Whereas P1 through P3 used generic inputs and were intended for evaluation simulations, P4 was set up to be applied to an actual site. P1 through P3 were used to develop and test the TRIM.FaTE algorithms. P4 was developed and used to illustrate and evaluate the likely limits of TRIM.FaTE with respect to the number of land parcels and length time steps used. This prototype had the shortest plausible time step (1 hours), a large number of land units in the plan view (20 parcels), and 21 different biotic domain types. This level of detail resulted in several hundred cells, including abiotic and biotic domain instances, and the sinks needed to account for transformation and transport losses outside of the system boundary. To test the model using a realistic ecosystem, P4 was applied to an area in the northwestern region of the United States. This prototype was developed as described in the setup methodology in Chapter 3.0. This section provides a general description of the P4 study area and the process of mapping the case study area into a form that is usable in TRIM.FaTE.

Description of Environmental Setting. In P4, the TRIM.FaTE model was applied to the simulation of B(a)P and phenanthrene releases in a much more realistic test case: a mixed use landscape surrounding an aluminum smelter. The circular region containing all land within 50 km of the facility was examined to define the boundaries of the study area. Precursory air dispersion modeling was performed and results indicated that significant impacts of the emissions occurred

within a radius of 5 km. The land use within this 5-km area was evaluated from Geographic Information System (GIS) information and it was determined that an oval study area approximately 8.5 by 9.0 km would provide an instructive test case for the TRIM.FaTE model. Figure 4-4 is the plan view and Figure 4-5 displays the cross-sectional views of the study area used for the test case.

The test case facility is located near a bay in an area that is predominantly industrial in nature. Much of the area immediately surrounding the smelter is used for storage of timber prior to ocean shipment. The nearest residents (human) are located approximately 800 meters east, north, and northeast of the facility. Approximately 800 meters north of the aluminum smelter is a ridge running in a southeast-northwest direction, with a maximum elevation of approximately 120 meters above sea level.

The only other major industrial facility in the vicinity of the aluminum smelter that has been identified as having a significant potential to emit air pollutants is a paper mill approximately 5 km due west of the smelter and on the bay. Nearby sources of polyaromatic hydrocarbons (PAH) may also include residential wood smoke, emissions from automobiles (to air), and boats (to water), among others. For purposes of P4, it was assumed that the aluminum smelter was the only source of phenanthrene and B(a)P within the study area.

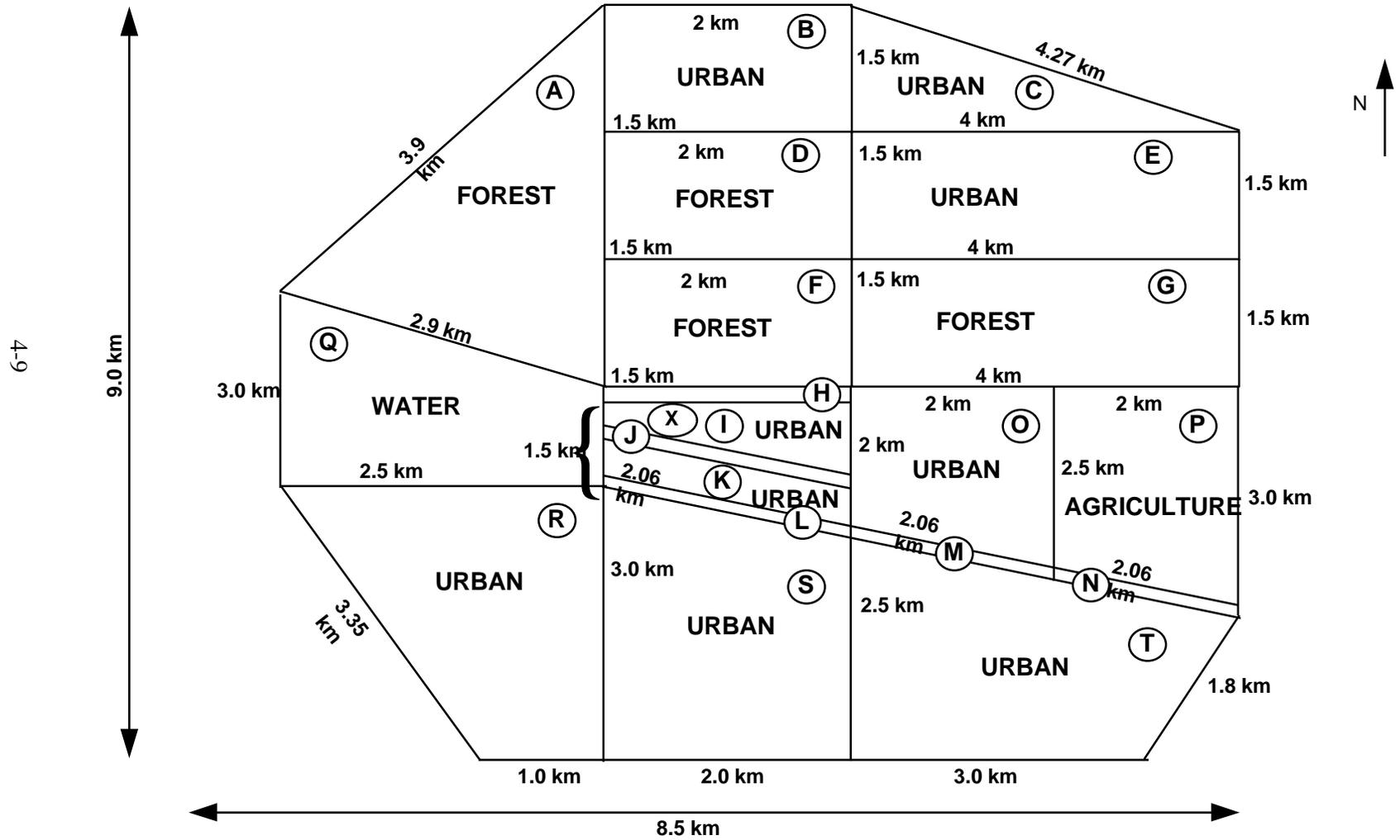
Although an actual location in the northwestern region of the United States was used as a rough guide for constructing this system, the application of TRIM.FaTE to this system was not intended to provide pollutant estimates for any existing facility in the United States.

Mapping the Ecosystem for P4. The plan view of the map resulting from the mapping process is shown in Figure 4-4. This process also involved setting up the domains and associated links as described in Chapter 3.0.

Determining the appropriate grid scale to use in this modeling effort is based on tradeoffs between the desired level of detail in the results and the data computational requirements necessary to run a detailed model. When determining the grid scale to use in the model, it is desirable to include as much detail as necessary to capture the spatial resolution, both in terms of land use and in order to capture the spatial change in chemical concentration. On the other hand, it is undesirable to have so much detail as to increase the complexity of the model to the point where it is difficult to set up and run. Ideally, there should be enough grids to capture the details needed for the required task and no more. Based on this tradeoff and as shown in Figure 4-4, the

Figure 4-4

Plan View for Study Area in Prototype 4

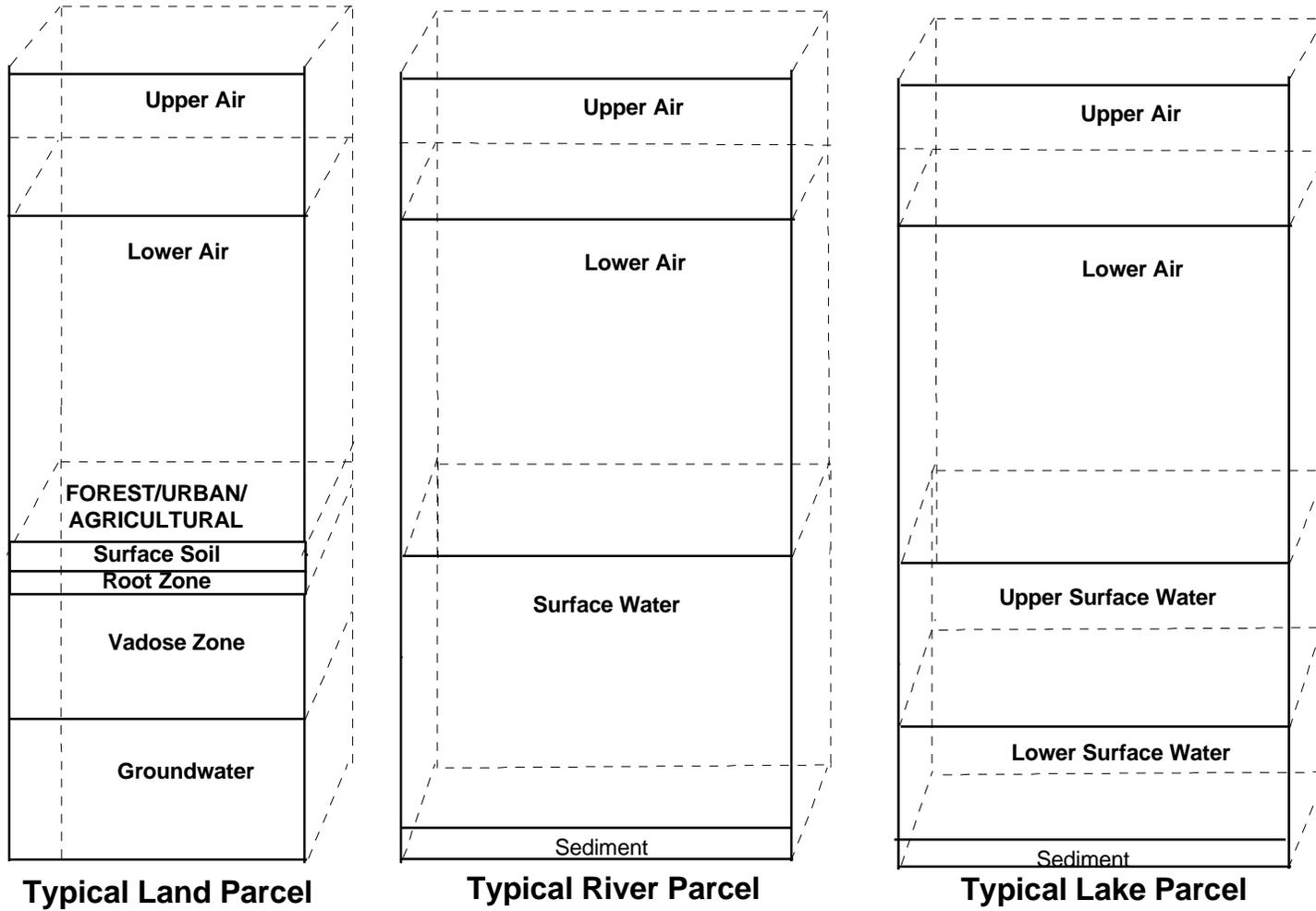


(X) Source

Figure 4-5

Cross Sectional View for Land, River, and Lake Parcels in Prototype 4

4-10



landscape was divided into 15 land units (parcels), and the water systems were divided into 5 water units (parcels). It is important to note that the embayment and other waters surrounding the smelter were assumed to be fresh, not saline, for purposes of the modeling effort.

The GIS data for this area indicates that the land area is primarily forest and urban, with a patch of agriculture and some very small parcels of grassy vegetation within the urban areas. GIS databases accessed to characterize the study area are summarized in Table 4-1. Details on each database are available in a separate report entitled *Draft GIS and Spatial Data Report for the Total Risk Integrated Model (TRIM)*⁴⁰. The pattern of land use is irregular and parcels were defined to be representative of the major land usage for the specific parcel selected.

Consequently, the location of each land use type does not correspond exactly with the actual location of that type of land, but the total area of each type of land is representative of the total actual areas. In locating the different land types, an effort was made to replicate the actual locations of each usage as much as feasible. The grids are either urban, forest, or agriculture. The small amount of grassy vegetation was accounted for by assuming that the urban parcels consist of grassy and paved areas.

4.3 Prototype Features

The specific features simulated in the prototypes are discussed in this section. Section 4.3.1 presents the types of abiotic domains modeled; Section 4.3.2 includes the types of biotic domains modeled; and Section 4.3.3 discusses the abiotic and biotic links associated with the prototypes.

4.3.1 Abiotic Domains

In P1 (Figure 4-1), the air, soil, and surface water each consist of a single volume element. Groundwater was simulated simply as a sink to the soil domain. P2, as shown in Figure 4-2, consists of an air domain that contained 4 volume elements (2 upper air and 2 lower air layers); the soil domain, which was divided into 4 volume elements (surface soil, root zone, and vadose zones 1 and 2); and groundwater, surface water, and sediment, which were each simulated as a single volume element. In P3, (Figure 4-3) the air domain consists of 6 volume elements (2 lower air and 2 upper air over soil, and a lower air and upper air over surface water); the soil domain was divided into 32 volume elements (8 surface soil, 8 root zone, 8 vadose zone 1, and 8 vadose zone 2); groundwater and surface water were both simulated with 2 volume elements; and sediment was simulated as a single volume element. P4 simulates 129 abiotic volume elements. As shown in Figures 4-4 and 4-5, parcels were defined and divided vertically based on domain type. The 129 abiotic domain instances associated with the parcels in P4 are summarized in Table 4-2.

Table 4-1

Databases Consulted in Developing Prototype 4 Ecosystem

Data type	Database	Characteristics of Database				
		Coverage	Data source	Scale	Attributes	Notes
Land use and land cover	USGS Land Use and Land Cover	National	High-altitude photographs	Minimum interval = 40 m to 160 m	Anderson detailed land use categories	Pros: Easily aggregated into general categories. Cons: Created in late 70s and early 80s (out of date). Long narrow polygons are precluded due to minimum width requirement.
Hydrology	Reach File	National	EPA	1:500K to 1:100K	Extensive	Pros: National in extent. Cons: Current version (RF1) not reliable for all areas of the country. Complex routing (e.g., flow direction not stated explicitly). RF3 file currently under development may be improvement.
Elevation	USGS 1 Degree DEM	National	Maps and photographs	70 m x 90 m cell size	Elevation of each cell as integer	Pros: National in extent. Highest resolution dataset available for whole nation. Cons: Accuracy low in areas of low relief. Cell size leads to smoothing of local relief.
Soils	State Soil Geographic database (STATSGO)	National	Soil survey maps, remote sensing	map unit = 625 hectares = 2500 m x 2500 m square; depth to 250 cm in 11 layers	percent-ages of soil types in each map unit (21 classes)	Pros: National in extent. Cons: Poor resolution. Not easily translatable for use in spatial models. No mapping below 250 cm depth. Sometimes discontinuous at state lines.

Table 4-2

Types of Abiotic Domains and Number of Volume Elements Modeled

Domain	Number of Volume Elements *			
	P1	P2	P3	P4
Air	1 - Air Layer	2 - Upper Air Layer 2 - Lower Air Layer	3 -Upper Air Layer 3 - Lower Air Layer	20 -Upper Air Layer 20 - Lower Air Layer
Soil	1 - Soil (general) 1 - Groundwater	1 - Surface Soil 1 - Root Zone 1 - Vadose Zone 1 1 - Vadose Zone 2 1 - Groundwater	8 - Surface Soil 8 - Root Zone 8 - Vadose Zone 1 8 - Vadose Zone 2 2 - Groundwater	14 - Surface Soil 14 - Root Zone 14 - Vadose Zone 1 14 - Vadose Zone 2 14 - Groundwater
Surface Water	1 - Surface Water Layer	1 - Surface Water Layer	1 - Upper Surface Water Layer 1 - Lower Surface Water Layer	1 - Upper Lake Layer 1 - Lower Lake Layer 5 - River Segments
Sediment	NA	1 - Interstitial Water 1 - Sediment	1 - Interstitial Water 1 - Sediment	6 - Interstitial Water 6 - Sediment
TOTAL NUMBER	4 Volume Elements	12 Volume Elements	44 Volume Elements	129 Volume Elements

*Reaction and advection sinks are not listed in this table.

4.3.2 Biotic Domains

In P1 and P2, a single fish species is modeled and only uptake and loss of contaminant through the gills is simulated. In the transition from P3 and P4, the number of biotic water column domain instances was expanded from a single fish species to an aquatic food web represented by several feeding trophic levels (domain instances). Bioaccumulation by herbivores, as well as omnivores and carnivores, is accommodated within the P3 and P4 simulations. It is important to note, however, that the trophic level representations were simplified to reflect primary uptake and loss from a single representative species from each trophic level. No natural variability specific to individual populations or communities is accounted for in P3. In P4, distribution ranges for parameters such as lipid content, ventilation rate, and individual size are included. For example, the aquatic carnivore community is represented by a single finfish, the Largemouth Bass.

Both P3 and P4 include terrestrial wildlife as domain instances. Wildlife may be exposed to contaminants through food, soil, and water ingestion, and through inhalation of contaminants in air. Elimination of contaminants from body tissues may occur through metabolic breakdown of the contaminant and excretion through urine, feces, milk (mammals only), and eggs (birds and reptiles only). Terrestrial and semiaquatic biota were not considered in P1 and P2. Two species were introduced in P3: a white-footed mouse (*Peromyscus leucopus*) and the belted kingfisher (*Ceryle alcyon*). These species were selected because they are taxonomically dissimilar (mammal versus bird) and represent differing domains (terrestrial omnivore and semiaquatic piscivore, respectively). P4 simulated a more complex terrestrial, aquatic, and semiaquatic system, as summarized in Table 4-3.

Table 4-3

Biotic Domains Modeled

Domain	P1	P2	P3	P4
Aquatic Ecosystem	<ul style="list-style-type: none"> • Single Fish Species 	<ul style="list-style-type: none"> • Single Fish Species 	<ul style="list-style-type: none"> • Macrophytes (Benthic Herbivores) • Aquatic Herbivores • Aquatic Omnivores • Aquatic Carnivores 	<ul style="list-style-type: none"> • Macrophytes (Benthic Herbivores) • Mayfly (Benthic Herbivores) • Bluegill (Modeled as Herbivore) • Channel Catfish (Omnivore) • Bass (Carnivore) • Mallard (Herbivore) • Raccoon (Omnivore) • Tree Swallow (Insectivore)
Terrestrial Ecosystem	NA	NA	<ul style="list-style-type: none"> • White-footed Mouse (Omnivore) • Earthworm (Soil Detritovore) • Plant Leaves, Roots, Xylem and Stem 	<ul style="list-style-type: none"> • White-footed Mouse (Omnivore) • Earthworm (Soil Detritovore) • Black-capped Chickadee (Insectivore) • Red-tailed Hawk (Predator) • Long-tailed Weasel (Predator) • Black-tailed Deer (Herbivore) • Long-tailed Vole (Herbivore) • Mink (Piscivore) • Trowbridge Shrew (Ground Invertebrate Feeder) • Insects • Plant Leaves, Roots, Xylem and Stem
Semi-Aquatic Ecosystem	NA	NA	<ul style="list-style-type: none"> • Belted Kingfisher (Piscivore) 	<ul style="list-style-type: none"> • Belted Kingfisher (Piscivore) • Wetland Plant Leaves, Roots, Xylem and Stem

P3 and P4 also simulated pollutant transfer to earthworms. The concentration in earthworms was assumed to be in equilibrium with the solid, liquid, and vapor-phase concentrations of the chemical in the root zone volume elements.

The plant domain was introduced to the TRIM.FaTE framework in P2. The plant component of the ecological model implemented for P2 and subsequent prototypes is comprised of leaves, roots, xylem, and stem. Plants are divided into these components (volume elements) because: (1) the literature suggests that concentrations of non-ionic organic contaminants in foliage are primarily related to those in air and that concentrations in roots are generally related to those in soil (with stems serving as the conduit between the two), and (2) herbivores may eat part but not all of a plant. The xylem is added for future versions of the model that may address exchanges between volume elements in which the xylem plays a critical role. Currently, each volume element is assumed to be homogeneously-mixed. The plant algorithms implemented in P2 through P4 are applicable for mature plants only, and do not yet address plant growth.

4.3.3 Links

If mass can move from one cell to another cell without first moving through intervening cells, then the two cells are considered "linked." Each linkage is associated with an algorithm that determines the direction and rate of mass flow between the two cells. Linkages may be between adjacent volume elements or within a volume element. At a given spatial location, and within a single volume element, more than one domain may exist and linkages may exist between these domains. The mass transfer algorithm specific to each linkage was based on review of the appropriate scientific literature and is discussed in detail in the technical support document¹.

Table 4-4 shows examples of generalized linkages applied to P1 through P4. This table is generic and can be used in conjunction with Tables 4-2 and 4-3 to define a specific link. For example, in P2 through P4, transfer of a pollutant can occur from an upper air cell to adjacent upper air cells and to a lower air cell. This is represented in Table 4-4 by the air (sending domain) to air (receiving domain) link. A more complex example is the links associated with the kingfisher from the semi-aquatic ecosystem. As a receiving domain, pollutant(s) can transfer to the kingfisher from air (i.e., lower air), soil (i.e., surface soil), surface water (i.e., upper lake layer), and aquatic (i.e., bluegill) ecosystems.

Table 4-4

Examples of Links Associated with Domains

Sending Domain	Receiving Domain
Air	Air Soil Surface Water Terrestrial Ecosystem Semi-Aquatic Ecosystem
Soil	Air Soil Groundwater Surface Water Terrestrial Ecosystem Semi-Aquatic Ecosystem
Groundwater	Groundwater Surface Water
Surface Water	Surface Water Sediment Aquatic Ecosystem Semi-Aquatic Ecosystem Terrestrial Ecosystem
Sediment	Surface Water Aquatic Ecosystem
Terrestrial Ecosystem	Terrestrial Ecosystem Air Soil
Aquatic Ecosystem	Aquatic Ecosystem Semi-Aquatic Ecosystem Terrestrial Ecosystem Surface Water
Semi-Aquatic Ecosystem	Terrestrial Ecosystem Air Soil Surface Water

The links from sending domains to sinks are not shown in Table 4-4. Sinks refer to the cells of pollutant mass leaving the ecosystem through a reaction or physical process(es). Section 4.4 describes these processes.

4.4 Fate and Transport Processes

One of the goals of the TRIM modeling framework was to develop underlying generalizations, or “rules” for algorithms or estimation techniques. During the development of the transfer factors, common rules underlying the development were observed and are presented in Appendix B. These rules are based primarily on the physics and chemistry of the underlying transport processes rather than on any attribute of specific domain pairs. For example, because transport from one cell to another always involves advection and/or diffusion processes, the mathematical form of abiotic transport has a similar format for all domain-instance pairs.

Primary processes used to simulate pollutant movement in the abiotic domains are diffusion and advection. These are key components of the overall transfer rates. The transport occurs both in the gas and liquid phase for organic chemicals.

In the biotic domain, equilibrium relationships describing processes like bioaccumulation and biomagnification were converted to a non-equilibrium form that could be used in the mass transfer equations.

An **advective** process is one in which a chemical is transported within a given phase that is moving from one cell to another (Mackay¹⁷ refers to this as a *piggyback* process, in which a chemical is “piggybacking” on material that is moving from one place to another for reasons unrelated to the presence of the chemical). Mathematically, all that is required to calculate the advective flux is the velocity of the moving phase, and the amount of the chemical that is in the moving phase. Examples of advective processes considered for transport of a chemical from the soil domain to the surface water domain are erosion of surface soil, runoff from surface soil, and recharge from groundwater.

In a diffusion process, a chemical is transported from one cell to another as a result of the magnitude and direction of the concentration differences between the two domain instances at the interface between the two locations. This means that the direction of flux is not necessarily constant with time. Estimates of effective diffusivity for a chemical species in gas and liquid-phase diffusion were used to estimate the diffusive transfer rates.

Reaction and transformation processes are modeled using either a specified reaction/transformation rate or transformation half-life. In all cases, the mass of chemical transformed in a given cell is assumed to be lost from the system. To make possible a complete mass balance for the

entire environmental system being modeled, this sink is modeled as an additional cell that receives input only from the particular cell.

Reaction transformation processes include such processes as biodegradation, photolysis, hydrolysis, oxidation/reduction, and radioactive decay. These are processes that transform a chemical species into another chemical species; they do not involve a change of location or a change of domain.

It is also possible that a chemical species transfers from one domain instance to another at the same location. Possible examples include the non-equilibrium transfer of a chemical from the fluid (liquid/gas) phases of soil to the solid phase, the uptake of a chemical by fish from water, or the uptake of a chemical by worms from soil. These processes do not involve a change of location or a change of chemical species. These processes are typically expressed in terms of the half-time to equilibrium. The half-time to equilibrium is typically measured in one direction, i.e., from water to fish or from soil to worm.

5.0 Test Case

This chapter presents data inputs and model results for various runs implemented in P4 for the test site described in Section 4.2.4. Because P4 is a culmination of the knowledge acquired from P1 through P3 and is capable of simulating these three cases, P4 will henceforth be referred to as the TRIM.FaTE prototype.

5.1 Data Inputs

The data inputs used in this analysis are described in detail in the technical support document¹. A summary of the data inputs is provided in this section. The advective flows of media that transport the chemical throughout the system are a critical factor in the application of the model. Advective flows include wind, precipitation, erosion, runoff, and surface water. To realistically model advective flows, site-specific parameters were used to the extent possible. Meteorological data for 1 year were obtained from a nearby airport. These data indicated approximately 80 centimeters of precipitation annually, an average wind speed of 5.8 meters per second (m/s), and a dominant wind direction toward the east. Soil properties were estimated with the assistance of GIS maps of the area. Surface water flow rates were estimated using local river flow data. Due to the absence of site-specific data for erosion and runoff flow, these parameters were estimated based on reasonable assumptions. An erosion rate of approximately 1 kilogram per square meter per day ($\text{kg}/\text{m}^2/\text{day}$) was assumed when precipitation occurs. This value is higher than would occur on a yearly average and is only used to demonstrate the type of results obtained. This estimate was made based on information obtained from a data set⁴¹, which indicated that there is 11 percent total soil loss for precipitation events less than 1.5 inches per hour. The runoff flow was estimated as 80 percent of the hourly precipitation rate.

For most species, the population sizes were estimated using information on the density of biota per area of habitat. For the purpose of investigating the possible impact of the biota on the distribution of chemical, biota were assumed to be located in all but the urban cells. Wildlife densities were assumed to be identical on forested and agricultural parcels of land.

5.2 Description of Model Runs

Using the assumed parameter values discussed previously, and those listed in the technical support document¹, numerous runs have been performed investigating the predicted behavior of the modeled system. For brevity, selective results are presented and analyzed in this section. The results reported here are categorized into three major divisions as follows:

- Theoretical phase calculations for predictive analyses (Section 5.3).
- Constant meteorological conditions (Section 5.4). This category consists of multiple runs under precipitation and no precipitation conditions
- Variable meteorological conditions (Section 5.5).

To highlight key features of the model, results for constant meteorological conditions are presented in greater detail than those obtained for variable conditions. By keeping meteorological conditions fixed, it is easier to discern key trends and responses of the model. For varying meteorological conditions, only the resulting apportionment of mass across the domains are compared and summarized at this time.

5.3 Results of Phase Calculations

As previously discussed, B(a)P and phenanthrene are assumed to be released from one source, an aluminum smelter, and initially there is no B(a)P or phenanthrene in the system. The general phase distribution of B(a)P and phenanthrene in abiotic media if equilibrium is assumed is shown in Table 5-1.

Table 5-1

Predicted Phase Distribution for B(a)P and Phenanthrene in Abiotic Media for Equilibrium

Domain Type	Sorbed		Dissolved		Vapor	
	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene
Air	9.7E-1	9.9E-1	0.0E+0	0.0E+0	3.3E-2	5.5E-3
Surface Soil	1.0E+0	9.9E-1	5.0E-5	8.5E-3	0.0E+0	0.0E+0
Surface Water	7.7E-1	2.0E-2	2.3E-1	9.8E-1	0.0E+0	0.0E+0
Sediment	1.0E+0	9.8E-1	1.5E-7	2.0E-5	0.0E+0	0.0E+0

Results presented in Table 5-1 calculated only from chemical properties of B(a)P and phenanthrene and the assumed properties of the media, indicate that B(a)P and phenanthrene will tend to be sorbed to solids. The main difference between B(a)P and phenanthrene concentrations is in surface water, where almost all of the phenanthrene is predicted to be dissolved. The fractions dissolved in sediment and surface water are approximately two orders of magnitude higher for phenanthrene than for B(a)P.

5.4 Results of Constant Meteorology Runs

Several test runs were performed to analyze the effects of precipitation and wind direction at steady-state conditions. A total of eight runs were performed, each using a constant wind speed of 5.8 m/s and a constant wind direction. Four of the runs did not include precipitation and had a wind direction from either the east, west, north, or south. The additional four runs included a precipitation scenario, with a wind direction from either the east, west, north, or south. An emission rate of 216 grams per day (g/day) for B(a)P and 17,600 g/day for phenanthrene resulted in different steady-state mass totals in the system for each run.

Results for runs with a due east wind direction are analyzed in detail in Sections 5.4.1 and 5.4.2 for purposes of discussing trends and model predictability relative to precipitation. A comparative analysis of these runs is presented in Section 5.4.3. The results from all runs under constant meteorological conditions are then compared and tabulated in Section 5.4.4. Separate discussions on the ecological components are presented in Section 5.4.5.

5.4.1 Results for No Precipitation, East Wind Direction Scenario

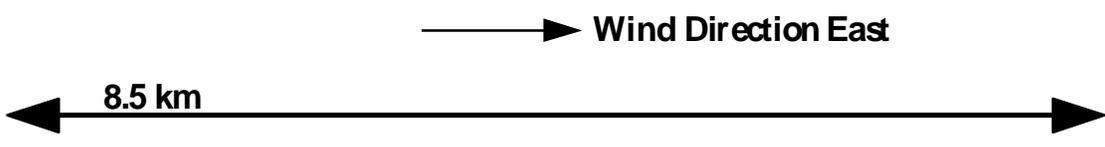
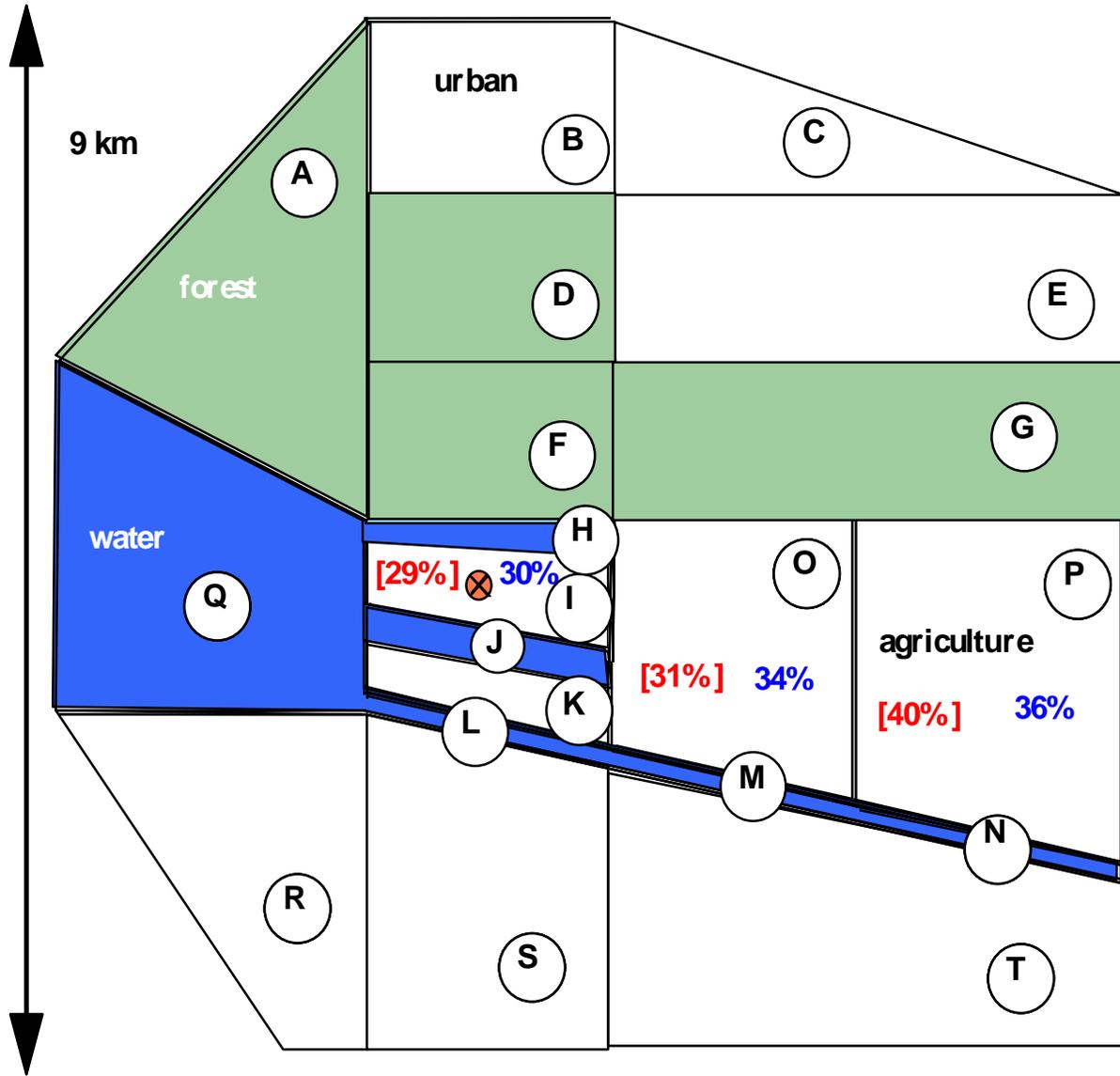
For a due east wind direction and the given location of the source term, there is transport mechanism by which the B(a)P or phenanthrene can enter the surface water if it is not raining. The B(a)P and phenanthrene emitted in parcel I can accumulate only in the parcel with the smelter or the parcels east of the facility (O and P). Because soil erosion or runoff is not assumed when precipitation does not occur, the B(a)P deposited to soil can only be resuspended or flow vertically through the soil layers. If resuspended, it is blown over the parcels to the east and/or out of the system. Almost no vertical flow in soil is predicted due of the sorption properties of B(a)P. The easterly wind flow will not bring the B(a)P over any surface water, and hence no dry deposition to surface water will occur.

Spatially, as shown in Figure 5-1, the B(a)P and phenanthrene in the system are partitioned relatively evenly among parcels I, O, and P, and there is an increase in the total mass of each chemical as one moves east from the facility. The mass per unit area of B(a)P and phenanthrene actually decreases as one moves east.

The presence of plants in parcel P (due to agricultural land use) is predicted to result in a magnification of the B(a)P in the parcel. This behavior can be seen by analysis of select transfer factors for parcel P (these transfer factors depend on the meteorological conditions and input parameters, but are independent of any source terms or initial conditions assumed). Analysis of the select transfer factors for parcel P (see technical support document¹) shows that the interaction of the

Figure 5-1

Predicted Steady State Spatial Distribution of B(a)P and Phenanthrene
 Wind Due East, No Precipitation



 Source
[xx%] - B(a)P
xx% - Phenanthrene
 Not to scale

air cell with the soil cell, directly and via the plants, accounts for more than 30 percent of the steady-state value of B(a)P in soil. This fraction is larger than the steady-state value in the plants themselves. Plants are thus predicted to be a magnifier of B(a)P in the system. Plants themselves accumulate only approximately 3 percent of the total B(a)P in the system, but approximately 10 percent of the B(a)P in the system is directly due to the flux from the plant to surface soil through litterfall. It can be seen from Figure 5-1 that 40 percent of total B(a)P is in parcel P (mostly in soil) (Figure 5-1), 30 percent of which is accounted for by the litterfall flux from the plants.

Table 5-2 summarizes the steady-state distribution of B(a)P and phenanthrene by domain type.

Table 5-2
Predicted Steady-State Results
(No Precipitation, East Wind Direction Scenario)

Distribution by Domain Type	B(a)P			Phenanthrene		
	Mass (g)	%	Normalized by Emission Rate (day)	Mass (g)	%	Normalized by Emission Rate (day)
Total in System	4.5e+03	100	4.6e+00	3.9e+04	100	2.2e+00
Air	2.1e+00	0.2	9.20e-01	2.0e+02	0.5	1.0e-02
Soil	1.0e+03	97.1	4.50e+00	3.8e+04	98.2	2.16e+00
Sediment	0.0e+00	0	0.00e+00	0.0e+00	0	0.00e+00
Surface Water	0.0e+00	0	0.00e+00	0.0e+00	0	0.00e+00
Plants	2.8e+01	2.7	2.00e-02	5.5e+02	1.4	3.00e-02
Non-Plant Biota	<0.05	<0.01	<4.6e-4	<4	<0.01	<2.2e-4

5.4.2 Results for Precipitation, East Wind Direction Scenario

The predicted steady-state spatial distribution of chemicals is more complicated when precipitation is occurring. When it is raining, there is enhanced atmospheric deposition, and erosion and runoff transport the chemical to neighboring soil and water cells. As shown in Table 5-3, most (98 percent) of the B(a)P is predicted to be in sediment (96 percent) and surface water (2 percent). Phenanthrene does not accumulate in sediment as much as B(a)P, and the total amount of phenanthrene in the system, when normalized by the emission rate, is 20 times smaller than that for B(a)P.

Table 5-3

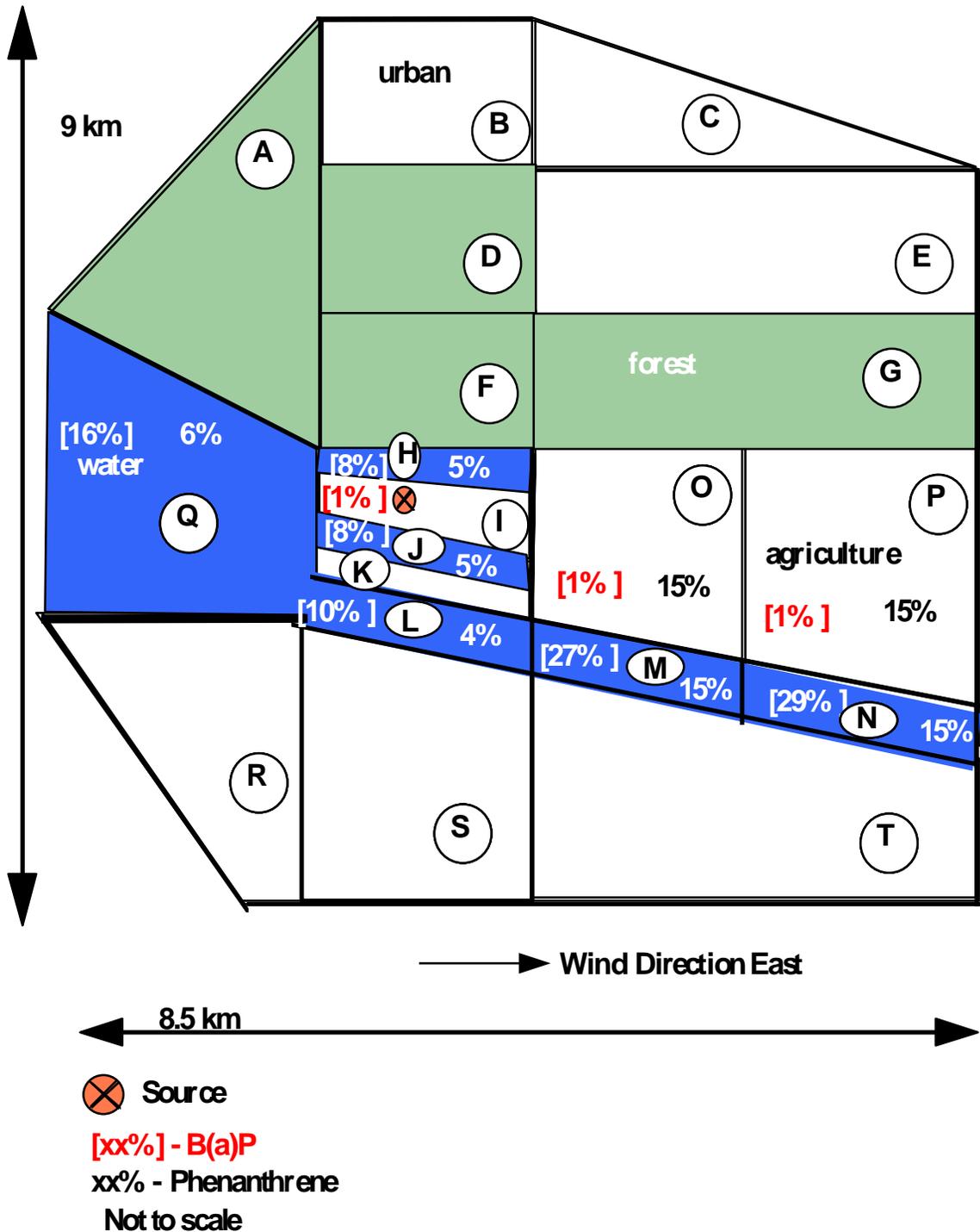
Predicted Steady-State Results (Precipitation, East Wind Direction Scenario)

Distribution by Domain Type	B(a)P			Phenanthrene		
	Mass (g)	%	Normalized by Emission Rate (day)	Mass (g)	%	Normalized by Emission Rate (day)
Total in System	4.5e+03	100	2.0e+01	1.5e+04	100	8.0e-01
Air	1.8e+00	0.04	8.0e-03	1.7e+02	1.1	8.8e-03
Soil	7.6e+01	1.7	3.5e-01	7.1e+03	47.3	3.50e-01
Sediment	4.3e+03	96.2	2.0e+01	5.1e+03	33.9	2.9e-01
Surface Water	7.6e+01	1.7	3.4e-01	2.3e+03	15.5	1.2e-01
Plants	1.8e+01	0.4	8.0e-02	3.0e+02	2.0	1.6e-02
Other	<0.2	<0.01	<2.0e-3	<0.15	<0.1	<8.0e-4

The spatial distribution of the chemicals is summarized in the Figure 5-2. The water bodies in M and N receive the chemicals through erosion from parcels O and P, respectively. The waterway in parcel L receives fluxes only through water flow from M. The water bodies north and south of the facility, parcels H and J, have the smallest amount of both chemicals; this is because the erosion from the parcel containing the smelter is split evenly between these two.

While much of the chemical is transported out of the system via wind or surface water outflow, cycles of movement within the system are predictable. This result is illustrated by the fact that, at steady-state, some mass of the chemical is predicted to be in the cells north of the facility, even though, due to the easterly wind direction, there is no direct interchange between the cell containing the smelter (parcel I) and the cells north of it. This results from the mass-balance nature of the model, as the cells to the north of the facility receive the chemicals through a chain of interdomain transfers. For example, the B(a)P emitted in parcel I is predicted to deposit in the soil cells east of the facility (parcels I, O, and P). After deposition, the B(a)P is advected via erosion into the waterways (H, J, M, and N), whereupon some is carried with the water flow into the water bodies L and Q. Some of this B(a)P is then predicted to diffuse into the air column above the water body. At this point, the chemical has been transported opposite to the wind direction, and will be blown back across the region containing the cells north of the smelter. Once deposited, it will undergo erosion and runoff back to the waterway H, to begin the cycle again. Such cycling cannot be predicted by models that do not fully integrate mass-balance across media. Environmental cycling, as discussed in Section 5.4.2, is expected under the precipitation

Figure 5-2
 Predicted Steady State Spatial Distribution of B(a)P and Phenanthrene,
 Wind Due East, Precipitation



scenario and is predicted by the simulation. For the no-precipitation, this is not expected or predicted.

5.4.3 Comparative Analysis

Using normalized emission rates to compare results, both meteorological cases predict B(a)P to accumulate in the environment more than phenanthrene. When precipitation is not occurring, most of the B(a)P accumulates in soil. There is a significant difference when precipitation is occurring due to accumulation in sediment. The difference between B(a)P and phenanthrene accumulation in sediment is due to the difference in their sorption properties (Table 5-1) and the difference of accumulation in soil is due to different half-life rates assumed (0.003/day for B(a)P and 0.006/day for phenanthrene).

The precipitation scenario results in a higher mass accumulation of B(a)P in the system than for the no precipitation scenario. The B(a)P mass in air, soil, and plants is higher in both magnitude and as a fraction in the system when there is no precipitation. This result indicates the importance of washout on the amount of B(a)P contained in these media and within the system.

Phenanthrene, unlike B(a)P, is predicted to accumulate more mass in the no precipitation scenario. The mass in air, soil, and plants is higher in magnitude when there is no precipitation. For the precipitation scenario, both the magnitude and fraction of mass in the system increased in the sediment and surface water.

5.4.4 Results for All Runs - Constant Meteorology

Tables 5-4 and 5-5 show the steady-state distribution of B(a)P and phenanthrene by domain type for different wind directions.

Qualitatively, almost all of the chemicals are predicted to be in soil or sediment, with the mass in sediment positively correlated with precipitation. The differences in the results for different wind directions are due to the spatial distribution of the domain types and assumed erosion and runoff flows.

When the wind is blowing north, the forest and urban cells north of the facility accumulate the chemicals in soil; the large fraction in soil in this case is due to the negligible erosion rates assumed for the urban cell farthest north from the facility. The summary results for the western and southern wind directions are similar; however, when the wind is blowing west, most of the

Table 5-4

**Predicted Distribution by Domain Type
(No Precipitation Scenario)**

Wind Direction	East		North		West		South	
Pollutant	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene
Total Mass in Ecosystem (g)	1000	3.9E+04	1100	3.3E+04	940	1.7E+04	8.8E+02	2.9E+04
Mass in system normalized by emission rate	4.6	2.2	5.1	1.9	4.4	0.9	4.1	1.6
Soil	97%	98%	84%	95%	44%	98%	80%	99%
Air	0%	0%	0%	1%	0%	1%	0%	1%
Surface Water	0%	0%	0%	0%	3%	1%	1%	0%
Sediment	0%	0%	9%	0%	54%	0%	19%	0%
Plants	3%	1%	7%	4%	0%	0%	0%	0%

Note: Non-plant biota is less than 0.1 percent of total mass in system.

Table 5-5

**Predicted Distribution by Domain Type
(Precipitation Scenario)**

Wind Direction	East		North		West		South	
Pollutant	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene
Total Mass in Ecosystem (g)	4.5E+03	1.5E+04	4900	1.2E+05	2500	7.2E+03	2500	9.9E+03
Mass in system normalized by emission rate	20.8	0.8	22.7	6.8	11.6	0.4	11.6	0.6
Soil	2%	47%	53%	95%	1%	41%	2%	52%
Air	0%	1%	0%	0%	0%	2%	0%	1%
Surface Water	2%	16%	1%	1%	4%	27%	3%	19%
Sediment	96%	34%	44%	2%	95%	30%	95%	28%
Plants	0%	2%	2%	2%	0%	0%	0%	0%

Note: Non-plant biota is less than 0.1 percent of total mass in system.

B(a)P is transported to parcels J and Q, while when the wind is blowing south, most of the B(a)P is transported to parcels L and Q. Since parcel J is located south of parcel I, it may seem unusual that B(a)P would be transported to parcel J when the wind is blowing due west; however, the B(a)P is homogeneously distributed in parcel I, and the wind speed from one cell to another depends on the angle of the boundary with respect to the wind direction.

For all wind directions except east, B(a)P is predicted to accumulate in sediment even in the absence of precipitation. In contrast, little phenanthrene accumulates in sediment unless precipitation is occurring. This difference is due to a combination of factors. First, the estimated transfer factors from air to water is approximately six times larger for B(a)P than for phenanthrene. This ratio is approximately the same as the ratio of the vapor-phase fraction of B(a)P (0.033) to that of phenanthrene (0.0055). This indicates that the diffusion to water from air is being predicted to be an important process. Another factor that accounts for these differences is that the reaction rate in water is approximately four times larger for phenanthrene than that for B(a)P. Finally, the calculated transfer factors for deposition of B(a)P to the sediment bed is more than 30 times larger than that for phenanthrene. This is due to the predicted phase distribution of the chemicals in the water body. Seventy-seven percent of the B(a)P is sorbed to suspended sediment, and hence is susceptible to deposition, while only approximately 2 percent of phenanthrene is sorbed.

5.4.5 Mass and Concentration Distribution in Biota

The mass distribution of B(a)P and phenanthrene within biota domains is based on steady-state conditions. The steady-state distributions of B(a)P and phenanthrene for four wind directions is shown in Tables 5-6 and 5-7 for conditions of precipitation and no precipitation, respectively. It should be noted that the mass distribution presented in these tables represent only the biotic portion of the total mass in the ecosystem. The mass in a particular biotic domain depends on the size of the population as well as its diet. A few general terrestrial and aquatic biota trends are discussed separately in the following paragraphs.

Most of the chemical mass is predicted to accumulate in plants when the wind direction blows towards the parcels containing plants. The mass in the system is highest when the wind is blowing north toward the forested areas, and lowest when blowing south toward the urban areas without precipitation. After plants, fish and macrophytes accumulate most of the B(a)P and phenanthrene. Relatively little of either chemical is predicted to accumulate in the terrestrial species, although terrestrial wildlife species that consume fish (e.g., raccoon) accumulate the most chemical mass. Note that this analysis is based on mass, not concentration. High concentrations of pollutants may be seen in some wildlife domains due to low population biomass.

Table 5-6

**Predicted Distribution in Biota by Domain Type
(No Precipitation Scenario)**

Wind Direction	East		North		West		South	
Pollutant	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene
Mass total (g) in Biota	2.84E+01	5.28E+02	7.36E+01	1.40E+03	4.27E-01	2.64E-01	1.06E-01	8.73E-02
Mass in system normalized by emission rate	1.32E-01	3.00E-02	3.41E-01	7.95E-02	1.98E-03	1.50E-05	4.93E-04	4.95E-06
Black-capped Chickadee	0%	0%	0%	0%	0%	0%	0%	0%
Redtailed Hawk	0%	0%	0%	0%	0%	0%	0%	0%
Tree Swallow	0%	0%	0%	0%	0%	0%	0%	0%
Mule Dee Blacktailed Deer	0%	0%	0%	0%	0%	0%	0%	0%
Longtailed Vole	0%	0%	0%	0%	0%	0%	0%	0%
Longtailed Weasel	0%	0%	0%	0%	0%	0%	0%	0%
Mink	0%	0%	0%	0%	0%	0%	0%	0%
Raccoon	0%	0%	0%	0%	0%	0%	0%	0%
Trowbridge Shrew	0%	0%	0%	0%	0%	0%	0%	0%
Mallard	0%	0%	0%	0%	0%	0%	0%	0%
Bluegill, Herbivore	0%	0%	0%	0%	3%	20%	3%	20%
Catfish, Omnivore	0%	0%	0%	0%	1%	1%	1%	2%
Largemouth Bass, Carnivore	0%	0%	0%	0%	69%	71%	70%	71%
Mice	0%	0%	0%	0%	0%	0%	0%	0%
Kingfisher	0%	0%	0%	0%	0%	0%	0%	0%
Insect	0%	0%	0%	0%	0%	0%	0%	0%
Insect, Mayfly	0%	0%	0%	0%	0%	1%	0%	1%
Macrophyte	0%	0%	0%	0%	27%	7%	26%	6%
Plant, Leaf	100%	100%	100%	100%	0%	0%	0%	0%

Table 5-7

**Predicted Distribution in Biota by Domain Type
(Precipitation Scenario)**

Wind Direction	East		North		West		South	
Pollutant	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene	B(a)P	Phenanthrene
Total Mass (g) in Biota	2.08E+01	3.03E+02	7.73E+01	1.93E+03	1.70E+00	8.09E+00	1.57E+00	9.52E+00
Mass in system normalized by emission rate	9.62E-02	1.72E-02	3.58E-01	1.10E-01	7.89E-03	4.59E-04	7.26E-03	5.40E-04
Black capped Chickadee	0%	0%	0%	0%	0%	0%	0%	0%
Redtailed Hawk	0%	0%	0%	0%	0%	0%	0%	0%
Tree Swallow	0%	0%	0%	0%	0%	0%	0%	0%
Mule Deer Blacktailed Deer	0%	0%	0%	0%	0%	0%	0%	0%
Longtailed Vole	0%	0%	0%	0%	0%	0%	0%	0%
Longtailed Weasel	0%	0%	0%	0%	0%	0%	0%	0%
Mink	0%	0%	0%	0%	0%	0%	0%	0%
Raccoon	0%	0%	0%	0%	0%	1%	0%	0%
Trowbridge Shrew	0%	0%	0%	0%	0%	0%	0%	0%
Mallard	0%	0%	0%	0%	0%	0%	0%	0%
Bluegill, Herbivore	0%	1%	0%	0%	3%	19%	3%	20%
Catfish, Omnivore	0%	0%	0%	0%	1%	2%	1%	2%
Largemouth Bass, Carnivore	5%	2%	1%	0%	69%	70%	70%	71%
Mice	0%	0%	0%	0%	0%	0%	0%	0%
Kingfisher	0%	0%	0%	0%	0%	0%	0%	0%
Insect	0%	0%	0%	0%	0%	0%	0%	0%
Insect, Mayfly	0%	0%	0%	0%	0%	1%	0%	1%
Macrophyte	2%	0%	0%	0%	27%	6%	26%	6%
Plant, Leaf	93%	97%	98%	100%	0%	0%	0%	0%

Concentrations in Terrestrial Biota. Estimated steady-state concentrations for B(a)P and phenanthrene in the terrestrial ecosystem are presented in Figures 5-3 and 5-4, respectively. The concentrations do not include background concentrations of the contaminants in any media. The wind direction in the scenario depicted is due north, and there is no precipitation. As previously stated, the emission rate for B(a)P is 216 g/day (1,000 g at steady-state), and the emission rate for phenanthrene is 17,600 g/day (39,000 g at steady-state). The concentration of B(a)P in surface soil (the top 1 millimeter) is approximately six orders of magnitude higher than that in root zone

Figure 5-3

Steady State Concentrations of B(a)P in Biota and Soil in a Forested Parcel, No Precipitation

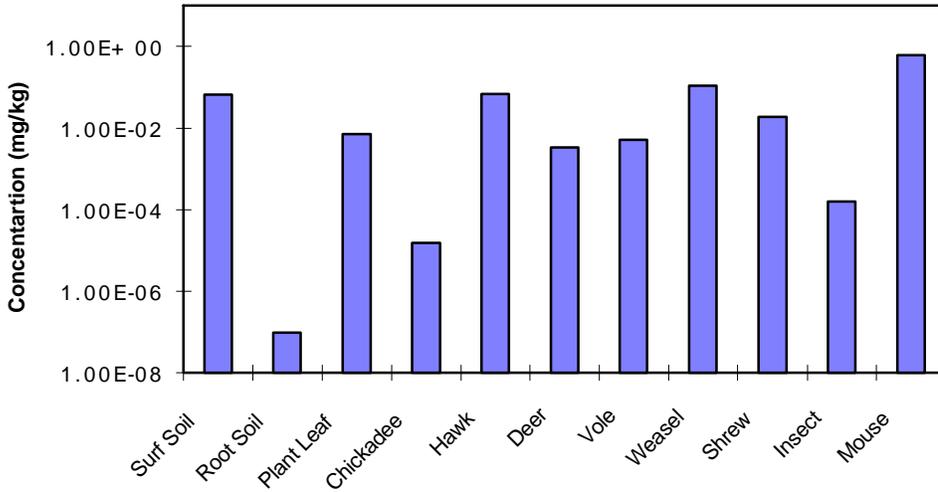
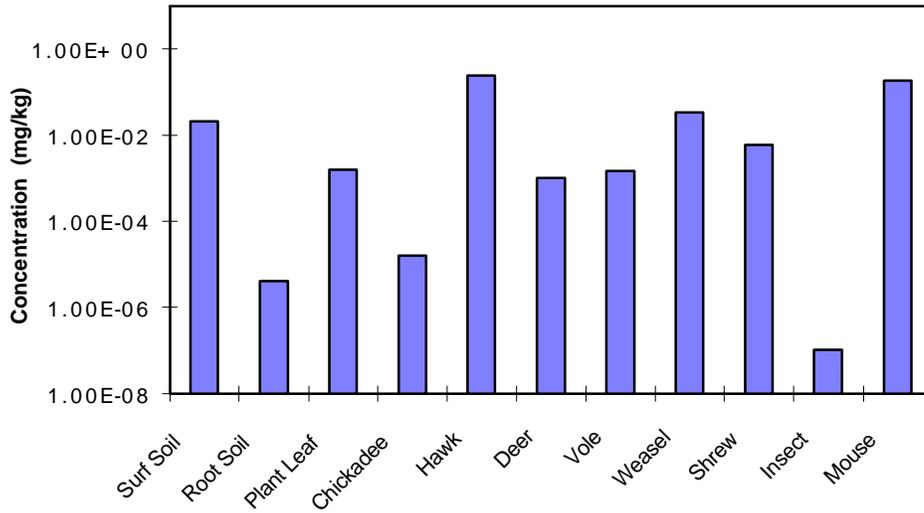


Figure 5-4

Steady State Concentrations of Phenanthrene in Biota and Soil in a Forested Parcel, No Precipitation



soil (the next 1 m) (Figure 5-3). The concentration of phenanthrene in root zone soil is substantially higher than that of B(a)P, as would be expected given the higher emissions rate of the former chemical.

Even though wildlife domains do not contribute significantly to the mass balance of PAHs, concentrations of the chemicals in wildlife are generally within two orders of magnitude of the concentrations in plant leaves and surface soil. The transfer from surface soil is the largest contributor to the mass in wildlife. Because of the large difference in contaminant concentrations in surface and root zone soil, the wildlife results are sensitive to the fraction of soil assumed to be incidentally ingested from each of these domains. Future modifications of the model will focus on improving the accuracy or expressing the uncertainty in the soil-to-wildlife transfers as represented here. Because of the low concentrations of PAH in earthworms and plant roots, these domains are not represented in the figures. For example, the estimated concentrations of B(a)P in earthworms and plant roots are 4×10^{-16} and 4×10^{-11} , respectively.

Despite the higher emission rate of phenanthrene, the estimated steady state concentrations of the chemical in individual domains are often lower than those for B(a)P. Specifically, the concentrations of phenanthrene in surface soil, plant leaf, deer, vole, weasel, shrew, and mouse are somewhat lower than those for B(a)P. The estimated concentration of phenanthrene in the insect is approximately three orders of magnitude lower than that of B(a)P in the insect.

Concentrations in Aquatic Biota. At this point in its development, TRIM.FaTE represents very simplified transfers between abiotic and biotic domains. Although the model is being tested on two PAHs emitted from an aluminum smelter located in a coastal northwestern setting, the aquatic system was assumed to be unstratified freshwater and not estuarine with complex salinity and density regimes. It was also assumed that the freshwater bluegill population would feed exclusively on plant matter (algae) and thus represent herbivorous creatures. In reality, these fish are omnivorous; however, they represented a suitable species to occupy the water column herbivore trophic level.

Table 5-8 shows the contribution to the steady-state values for the fish species in the water body in parcel Q. Comparing the mass normalized by emission rate, more B(a)P than phenanthrene is predicted to accumulate in all fish species. For carnivores and herbivores, the dominant uptake pathway is through interaction with the water column for both chemicals. There is a marked difference in the accumulated mass of each chemical for the omnivores (catfish). Most of the

B(a)P is accumulated from the sediment, while most of the phenanthrene is taken up through the water column.

Table 5-8

**Uptake Fractions for Specialized Fish Domains in Parcel Q
(Precipitation, East Wind Direction Scenario)**

Species	Uptake Fractions (% of total in specialized domain)	
	B(a)P	Phenanthrene
Carnivore (Largemouth Bass)		
Normalized mass of chemical in fish (g/g emission/day)	2.0E-3	5.6E-5
Water	61	86
Herbivore	38	14
Omnivore	1	0.2
Herbivore (Bluegill)		
Normalized mass of chemical in fish (g/g emission/day)	9.7E-5	1.6E-5
Water	97	100
Macrophyte	3	0
Omnivore (Catfish)		
Normalized mass of chemical in fish (g/g emission/day)	1.2E-5	6.8E-7
Water	1.3	90
Sediment	99	9
Herbivore	0.1	1
Macrophyte	0.1	0

It is also important to note that the distribution within biotic domains of B(a)P and phenanthrene predicted by the model suggests a surprisingly high percentage of PAH mass concentrated within the carnivorous largemouth bass (*Micropterus salmoides*) population as opposed to the other terrestrial and aquatic receptors (Tables 5-6 and 5-7). A detailed description of the assumptions and algorithms adopted for the aquatic transfers are provided in the technical support document¹. A few factors contributing to the apparent imbalance in PAH distribution among biotic receptors include diet and associated biomagnification tendencies, as well as the fact that the model segment Q was assumed to be a large lake or slow-moving embayment with a significant bass population of 50 to 100 individuals per hectare. While this density range is supported in the

literature for slower moving waters such as lakes⁴², when combined with lipid level estimates and assumptions of 80 percent of its diet being bluegills, the bass is inaccurately being predicted as the ultimate biotic sink. Further sensitivity analysis on the model and subsequent adjustments should result in a more accurate prediction of PAH distribution within the aquatic biota domains.

In addition, Table 5-8 indicates that the bottom-dwelling catfish uptakes 99 percent of its B(a)P from the sediment. Given the partitioning characteristics of B(a)P and the bottom-scouring habits of catfish, this may be fairly accurate. This uptake is driven by the assumption that 96 hours are required to reach steady state, as described in the technical support document¹. This assumption may be inaccurate; the sensitivity of the model estimates to this assumption will be tested in subsequent model runs.

5.5 Variable Meteorology

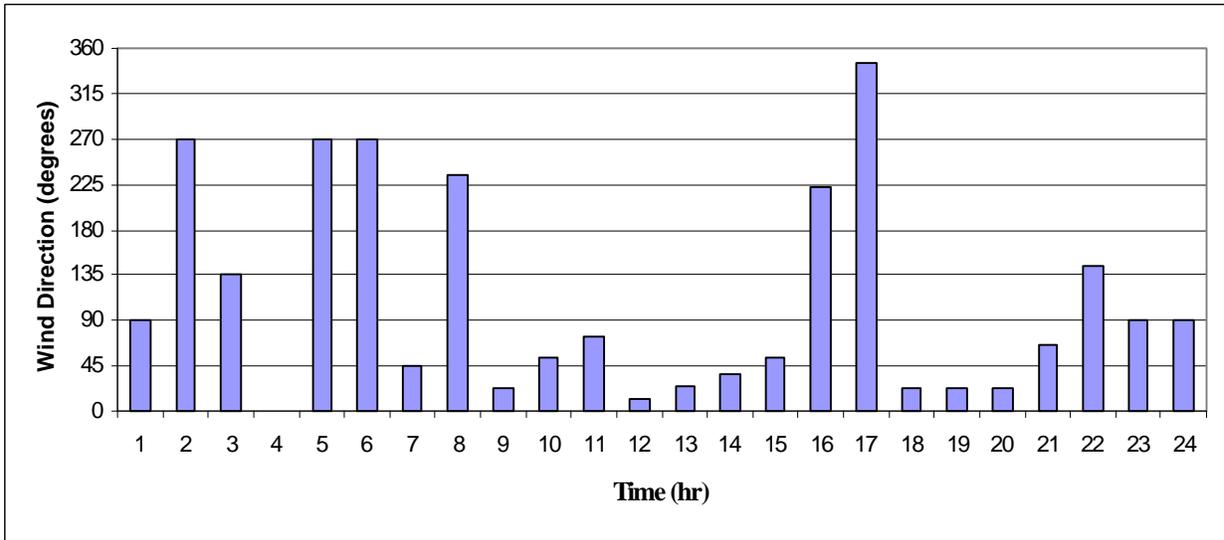
In this Section, the results for time-dependent meteorology are discussed. The emitted chemical is modeled for a 24-hour period. The factors that depend on time are the wind speed, wind direction, and precipitation. The wind direction and precipitation time profiles used in this analysis are shown in Figures 5-5 and 5-6.

Figures 5-7 through 5-10 show the predicted mass of each chemical in various domain types for the variable meteorological conditions. After 12 hours, each chemical is predicted to begin accumulating to some degree in almost all domain types. An exception to this is seen for phenanthrene in surface water. When precipitation stops (starting approximately the 19th hour), there is no longer any erosion or runoff load to the water bodies. It can be seen in Figure 5-8 that phenanthrene mass in SW starts decreasing marginally. At this point, the phenanthrene in the water bodies begins to either settle into the sediment or be flushed out, eventually reaching the outflow sink for the water domain in parcel Q.

The air domain is predicted to be most sensitive to the hourly fluctuations in meteorological conditions. This can be seen by looking at the first few hours, where the rapidly fluctuating profile of precipitation is reflected in the clearly observable oscillations in the chemical mass in the air domains (Figure 5-8). When precipitation is occurring, the chemical is removed from the atmosphere; when precipitation is not occurring, less chemical is removed, resulting in the small "peaks" during the second and fourth hours. After the fourth hour, the precipitation rate, when precipitation occurs, is lower than that in the first four hours. This results in smaller oscillations. Further, the chemical in the air domains will begin cycling as the wind direction changes from hour to hour.

Figure 5-5

Wind Direction (degrees) Profile for TRIM.FaTE Prototype



Clockwise from Due North Towards Direction of Wind

Figure 5-6

24-Hour Precipitation (mm/hr) Profile for TRIM.FaTE Prototype

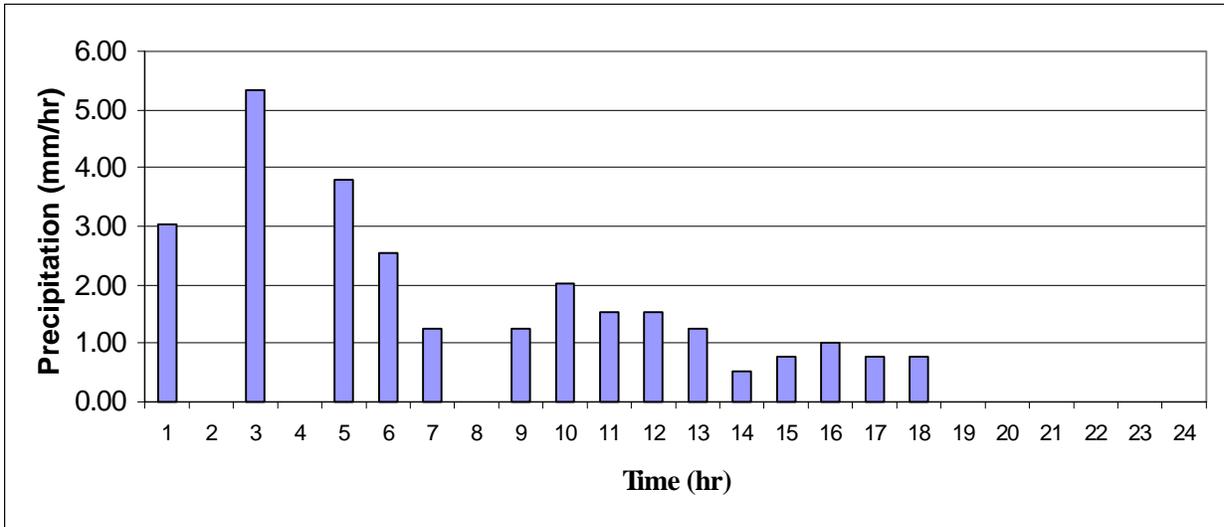


Figure 5-7

B(a)P Fraction of Mass Distribution for Parcels in TRIM.FaTE Prototype, Variable Meteorological Conditions

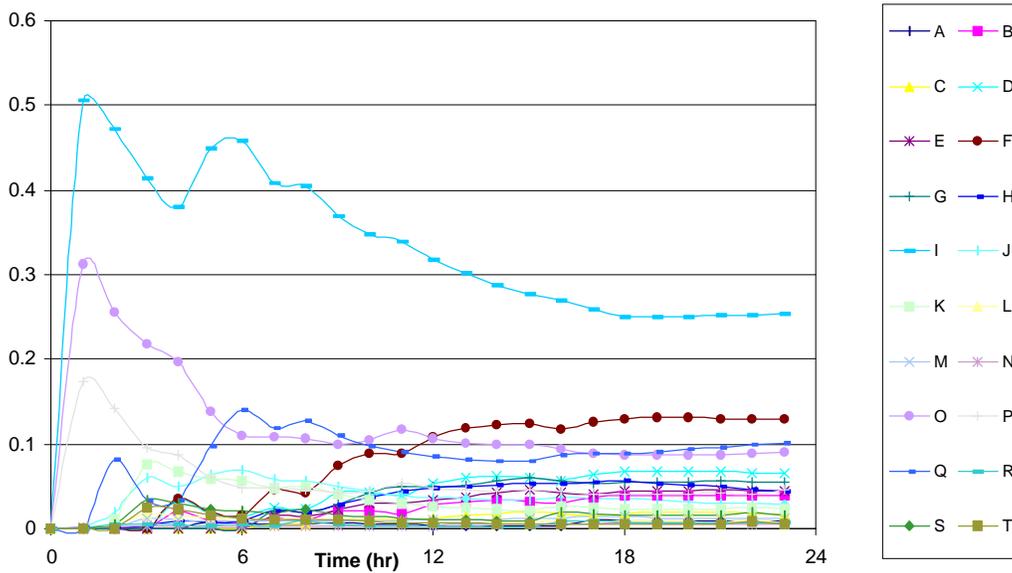


Figure 5-8

Phenanthrene Mass Distribution for Select Domains in TRIM.FaTE Prototype, Variable Meteorological Conditions

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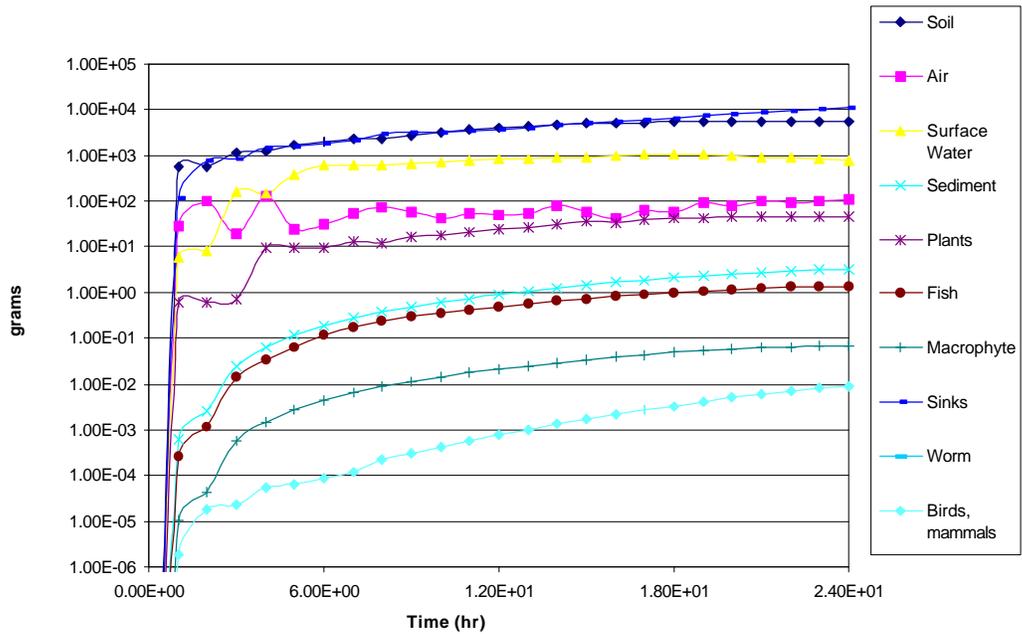


Figure 5-9

Phenanthrene Fraction of Mass Distribution for Parcels in TRIM.FaTE Prototype, Variable Meteorological Conditions

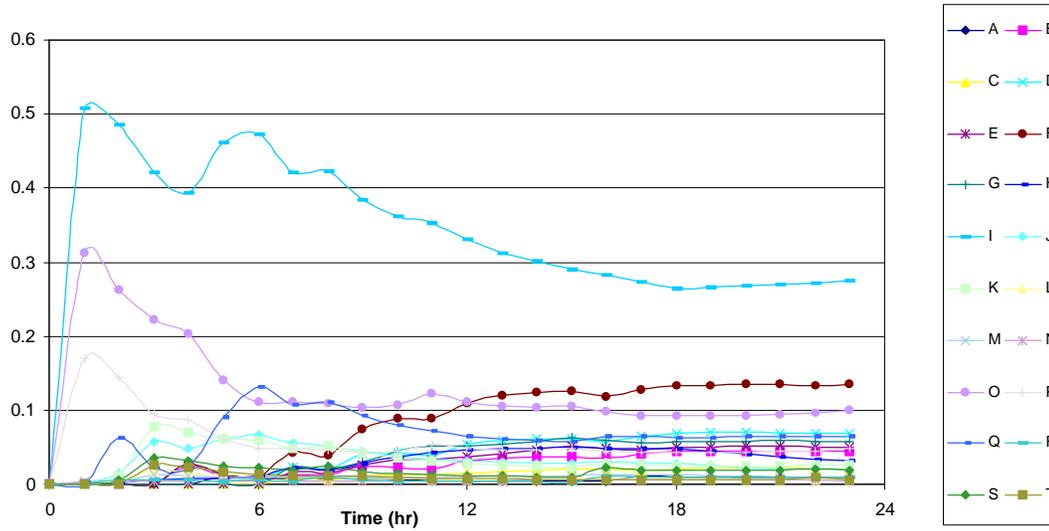
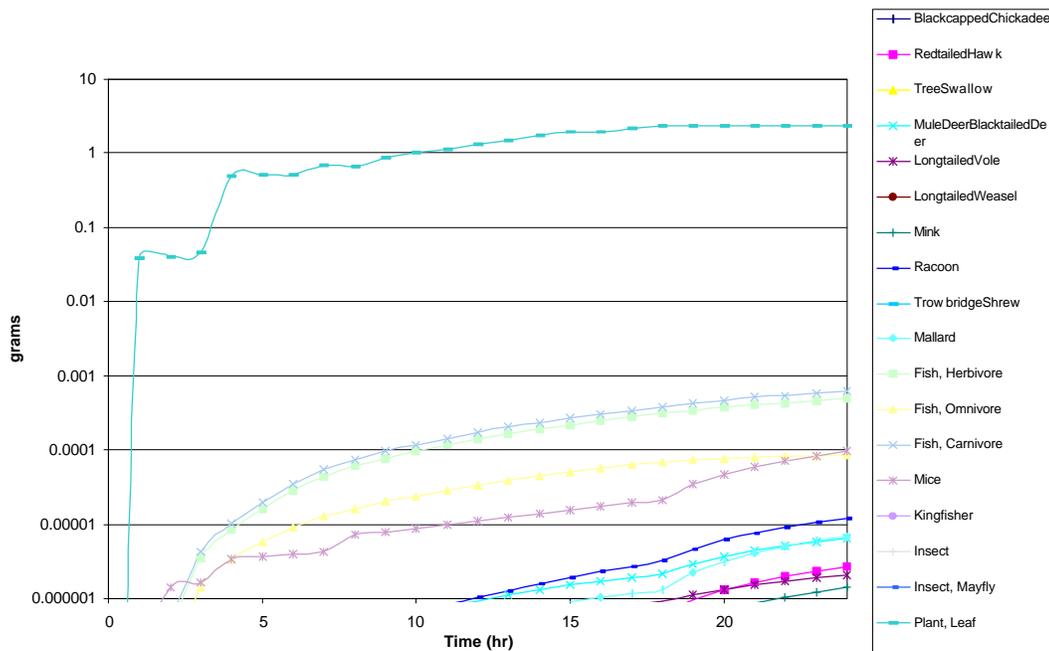


Figure 5-10

B(a)P Mass Distribution in Biota for TRIM.FaTE Prototype, Variable Meteorological Conditions



The plant domains are predicted to have a noticeable increase in chemical mass at the fourth hour (Figure 5-10). This is a result of the wind blowing north for the first time, as most of the plants are located north of the facility. The increase is more gradual for later hours. Similarly, there is a sharp increase for the aquatic domains (water column, sediment, fish) during the first few hours (Figure 5-10), with the mass in sediment and fish following the same general trend as that of the water column. There is comparatively little chemical mass predicted to accumulate in the biotic domains.

6.0 Evaluation of TRIM.FaTE

As a process for iterative discovery, science does not reward advocates; it rewards those who find truth. Many models are assembled through dialectic interactions among advocacy groups, i.e., those who favor complex models versus those who favor simple models; those who want to represent the highest plausible exposure versus those who want to represent central tendency; those who favor an environmental perspective versus those who favor an industry perspective, etc. TRIM and TRIM.FaTE aspire to a science-based model process, which requires that the goal be to model what is real. If the reality is that exposure cannot be modeled without large uncertainties, then this should be reflected in the model process. TRIM is designed to provide EPA and other users with a tool that can be used in a flexible and iterative manner to explore human and ecosystem exposures and provide insight in addition to risk estimates. The statistician George Box has noted that “All models are wrong, but some models are useful”⁴³. To make TRIM “useful” and scientifically defensible, it has been designed with flexibility, iterative analyses, and explicit treatment of sensitivity and uncertainty as core components of the model building and model implementation process.

In this chapter, conclusions and evaluations based on the current work on TRIM and TRIM.FaTE are provided. The chapter is divided into five major sections that compare the TRIM.FaTE prototype to other multimedia models; identify the capabilities, limitations, and important sensitivities of the current TRIM.FaTE prototype; and summarize the important conclusions that derive both from prototype development process and from the application of the prototype to a study site.

6.1 Comparison with Other Models (SimpleBOX and CalTOX)

To compare the results of TRIM.FaTE to other models, for illustrative purposes, two models were applied with the same landscape and chemical input data that were used for the TRIM.FaTE model case study. The models used for this comparison were CalTOX (Version 2.3)²³ and SimpleBOX (Version 2.0)²⁶. Comparisons among the three models were made for the distribution of mass in multiple environmental media for the chemicals B(a)P and phenanthrene. The descriptions of CalTOX and SimpleBOX are provided in Section 3.1.

To make the comparison tractable, and to make TRIM.FaTE results consistent with the type of information produced by the much less complex CalTOX and SimpleBOX models, an emission rate of 9 g/day to the air compartment of the case study site was considered. A steady-state mass distribution was obtained from each model

Figures 6-1 and 6-2 compare the results of mass distribution predictions for B(a)P and phenanthrene obtained for similar landscape data sets using CalTOX, SimpleBOX, and TRIM.FaTE.

From Figure 6-1, it can be seen that for B(a)P, TRIM.FaTE, SimpleBOX, and CalTOX all give similar distributions of mass in soil, water, sediment, and plant compartments. In the air compartment, TRIM.FaTE and CalTOX produce similar results and SimpleBOX is a factor of 10 lower. The results in Figure 6-2 show that for phenanthrene, which has a higher vapor pressure than B(a)P, all three models give similar distributions of mass in soil. For water and sediment, TRIM.FaTE and CalTOX produce similar results. For air and plants, all three models appear to yield a large variation in results. This variation appears to be due in large part to the differences in air/plant uptake factors among the models. This comparison indicates that TRIM.FaTE yields similar results to CalTOX and SimpleBOX for some media, but different results for others, based on different algorithms. However, without actual measured concentrations in a controlled system, it cannot be determined which model more accurately reflects reality.

6.2 Sensitivity Analysis for TRIM.FaTE

Five factors that determine the precision or reliability of an environmental transfer model are⁴⁴: specification of the problem (scenario development); formulation of the conceptual model (the influence diagram); formulation of the computational model; estimation of parameter values; and calculation and documentation of results, including uncertainties.

It should be recognized that there are some important inherent uncertainties in the TRIM.FaTE multimedia approach. Parameter uncertainties and model sensitivities are addressed in detail in the technical support document¹.

At this time, only a simplified sensitivity analysis for TRIM.FaTE has been completed. The method used considers the range of uncertainty in the parameter value and the linear elasticity of predicted organism concentration with respect to each input parameter. This method identifies parameters with both relatively high sensitivity and a large range of uncertainty. The method is used to identify parameters for which decreasing uncertainty would have the largest impact on reducing output uncertainty.

Figure 6-1
Model Comparison for B(a)P

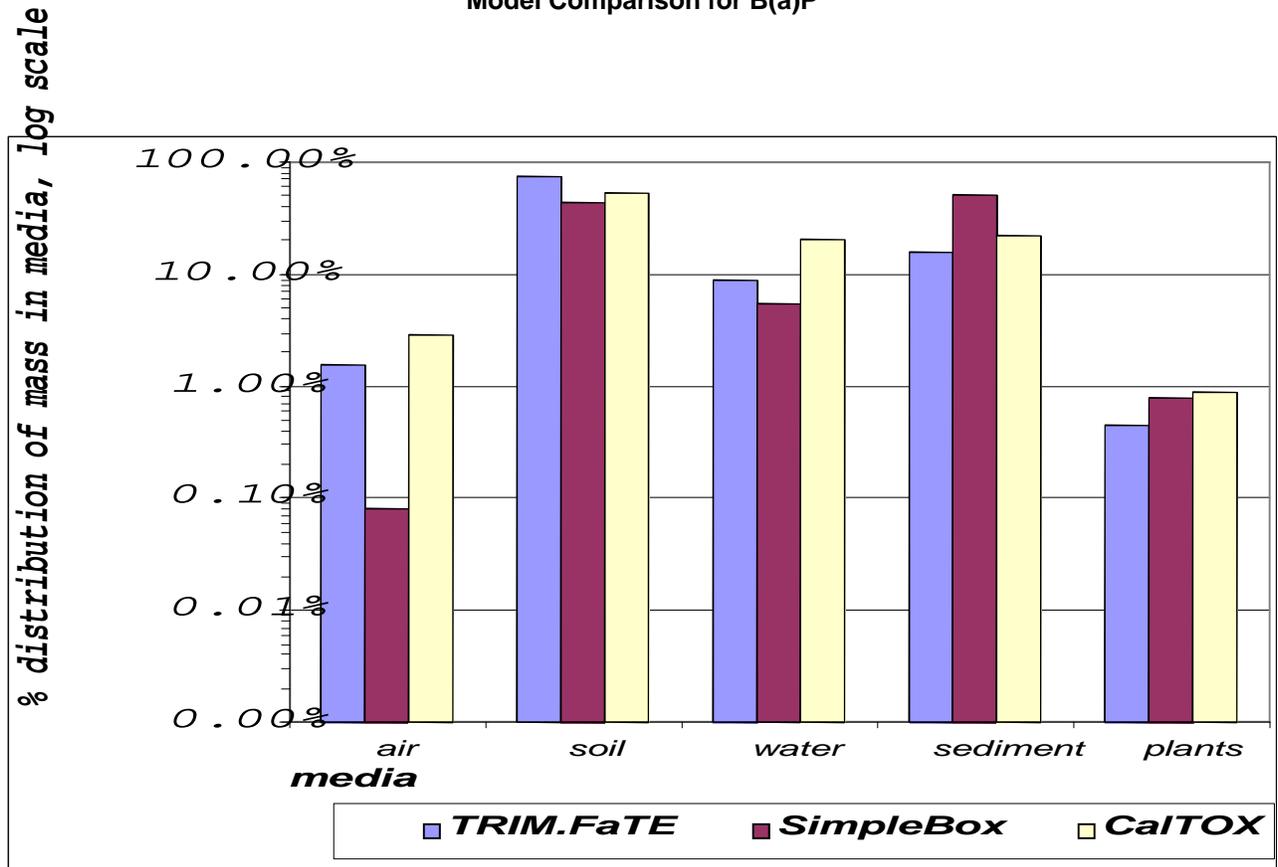
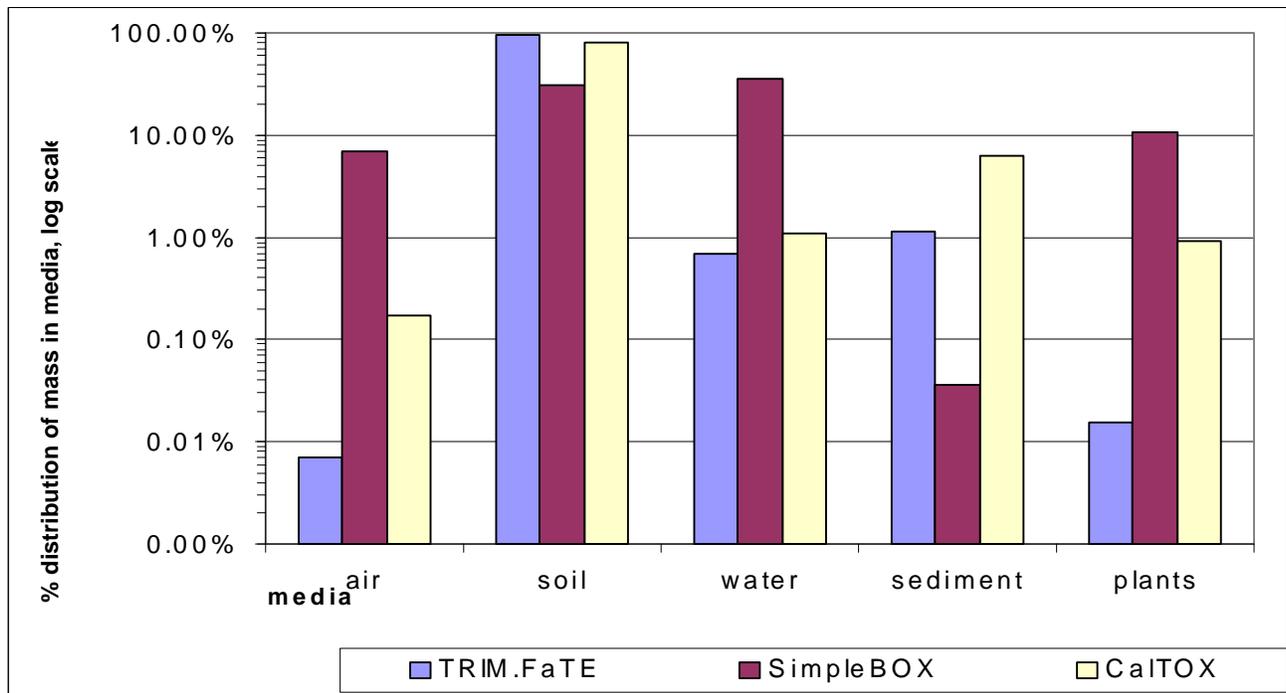


Figure 6-2
Model Comparison for Phenanthrene



The technique used in this preliminary method uses a sensitivity score, defined as:

$$\text{sensitivity score} = \frac{\partial Y}{\partial X_i} \times CV_i \frac{X_i^o}{Y^o}$$

where:

$$\begin{aligned} \frac{\partial Y}{\partial X_i} &= \text{change in output Y per change in input X} \\ CV_i &= \text{coefficient of variation of } i^{\text{th}} \text{ input} \\ X_i^o/Y^o &= \text{ratio of nominal values of input and output.} \end{aligned}$$

The sensitivity score was calculated for all of the inputs to the TRIM.FaTE model, and the sensitivity to the change in inputs was determined for the following outputs: chemical concentrations in a carnivorous fish, macrophytes, a vole, a chickadee, and a hawk. The calculation was made for B(a)P in a steady-state condition. The coefficients of variation used were estimated based on both reasonable judgment and coefficients of variation developed for the California EPA for similar parameters used in the CalTOX model. Of the 400 inputs, Table 6-1 presents the 20 inputs that have relatively large sensitivity scores.

As discussed in Section 5.4.5, the mass distribution in the carnivorous fish (bass) was predicted to be unusually high. The results of this analysis shows that the parameters with high sensitivity scores for the macrophytes and fish appear to be reasonable, relative to our expectations. B(a)P binds to particles in the air; therefore, exposure is influenced by how much B(a)P is transported to the surface water during wet deposition, based on the wash-out ratio, thus increasing the surface water concentration. Parameters that influence the concentration in the surface water also have a strong effect on the results because aquatic exposure is through surface water. Decay constants are highly uncertain because the model is sensitive to the decay content and the effects of varying them score high. B(a)P is likely to partition into the organic carbon in suspended sediment in water; thus, the amount of organic carbon suspended in water is an important factor. The carnivorous fish is also dependent on sediment properties, as its food comes primarily from the sediment. The assimilation efficiencies are highly uncertain for wild species.

Table 6-1

Parameters with High Sensitivity Scores for B(a)P

Parameter	Carnivorous Fish	Macrophytes	Chickadee	Vole	Hawk
Washout-ratio			x	x	x
Octanol-water partition coefficient	x	x			
Organic carbon partition coefficient	x	x	x		
Decay constants in air	x	x	x		
Decay constants in surface water	x	x	x		
Decay constants in sediment	x	x			
Decay constants in fish	x	x			
Suspended sediment in surface water	x	x	x		
Organic carbon in suspended sediment	x	x	x		
Sediment organic carbon fraction	x				
Porosity of sediment zone	x				
Assimilation efficiencies	x	x	x	x	x
Accumulation factor	x	x			
Fraction of lipids in fish	x				
Fish diet	x				
Water ingestion rate for the chickadee			x		x
Inhalation rate of the chickadee			x		x
Water ingestion rate of the vole				x	x
Food ingestion rate of the vole				x	x
Inhalation rate of the vole				x	x

The parameters with high sensitivity scores for the three terrestrial species (chickadee, vole, and hawk) included many of the same parameters as the aquatic species. The terrestrial species are sensitive to the chemical concentration in the surface water because they use the surface water in large part as their drinking water supply. The hawk also eats fish, whose chemical concentration is dependent on the concentration in surface water. Additionally, the chickadee and hawk are sensitive to the water ingestion rate and inhalation rate of the chickadee. The chickadee is obviously sensitive to its own intake rates, but the hawk is also sensitive to them

because it feeds on the chickadee. Similarly, both the vole and hawk are sensitive to the water ingestion rate, food ingestion rate, and inhalation rate of the vole.

The model results were found to be highly dependent on the chemical properties of the chemical species being modeled. Nonetheless, in all cases, the model was very sensitive to source terms. All model predictions were directly proportional to the initial inventory or input rates used. For many applications of a model such as TRIM.FaTE, source data are variable and/or uncertain, particularly for contaminant measurements in soils. For most chemicals, the model is sensitive to the magnitude of the transformation rates in soils, air, surface water, and/or sediment. These rate constants can have a large impact on the predicted persistence of any chemical species and are often the most uncertain inputs to the model. For volatile chemicals, the model is sensitive to the magnitude of the air-water partition coefficient. For semivolatile chemicals and inorganic species, the model is more sensitive to the soil-water partition coefficients. Researchers typically assume that these partition processes are linear and reversible. When this assumption is not valid, the reliability of the model is reduced because of the uncertainties about the degree to which soil partition processes diverge from ideal behavior. The transformation of contaminants in the environment can have a profound effect on their potential for persistence.

6.3 Overall Capabilities

TRIM.FaTE is a model that explicitly represents time and spatial resolution by the number of cells and links among its compartments. In descending order of reliability, the model will be capable of handling non-ionic organic chemicals, radionuclides, fully dissociating organic and inorganic chemicals, and solid-phase metal species. Limitations in reliability derive from relevance and availability of data. With careful attention to inputs and selection of the appropriate algorithms, the mathematical structure of TRIM.FaTE can be used to model partially dissociated organic and inorganic species. As better data and scientific understanding become available, TRIM.FaTE will be capable of assessing such difficult-to-model agents as surfactants, inorganic chemical species with high vapor-pressure-to-solubility ratios, and volatile metals. As a result, TRIM.FaTE will be applicable to most chemicals of concern from a multimedia, multipathway perspective.

6.3.1 Time Scales

The TRIM.FaTE model was designed to be applied over time periods ranging from 1 hour to 1 or more days, months, or years, when seasonally and yearly averaged partition factors apply.

6.3.2 Spatial Scales

Spatial resolution is implicitly linked to the time-step size selected. When short time steps are selected, TRIM.FaTE can provide spatial information on scales of hundreds of meters. The assumption that compartments are well-mixed requires that compartment dimensions be less than the distance traveled by a chemical in

one time-step. Because TRIM.FaTE is a compartmental-type model, there are no explicit vertical or horizontal dimensions in the cells used to represent various components of the environment.

In addition to the time-step considerations, other factors should determine the appropriate horizontal cell size. These include: (1) resolution of input datasets and (2) similarity of habitat (e.g., vegetation cover) and soils within a cell.

6.3.3 Chemical Classes

There are many classes of chemicals that must be addressed in environmental transport/transformation models, including organic chemicals, metals, inorganic chemicals, and radionuclides. These chemical species can also be categorized according to the physical state in which they are introduced to the environment (gas, liquid, or solid), according to whether they dissociate in solution (ionic or nonionic), and the charge distribution on the molecule (polar or nonpolar). The traditional fugacity-type approach is most appropriate for nonionic organic chemicals in a liquid or gaseous state. However, with modifications for condensation of solids on air particles, this approach can be made appropriate for solid-phase organic chemicals. Additional adjustments make possible the treatment of inorganic species, metals, and fully ionized organic species. Metals (such as mercury) and inorganic chemicals with a relatively large vapor pressure pose special problems not addressed in most multimedia models, but TRIM.FaTE provides the potential for addressing such species. In addition, TRIM.FaTE can handle special modeling problems, such as those that occur with mixed polarity and dissociating organic species, such as surfactants.

6.4 Limitations

TRIM.FaTE is being designed to simulate pollutant movement within these complex ecosystems. Given the complexity of processes dictating the transfer of pollutants within these systems, it must be understood that the model's predictive capability is presently limited to gross transfers of pollutants between sources, receptors, and sinks. The model's overall predictive capabilities depend on: (1) the explicit transfer links built into the model; (2) available databases for which it is possible to derive distributions of parameters; and (3) the current understanding of ecological and abiotic transfers.

The model is designed to accommodate new information in scientific understanding, so that its precision and usefulness will improve with time. Factors that contribute to the uncertainty in outputs of TRIM.FaTE include:

- Limitations on the number of receptor species representing terrestrial and aquatic trophic levels and the mass (number) associated with those species;
- Limitations on our understanding of pollutant synergistic interactions, and their effect on transfer, uptake, and loss rates;

- Limitations on our understanding of pollutant biotransformation processes and our ability to quantify such processes;
- Limitations on our understanding of biotic interactions at the population, community, and ecosystem level;
- Limitations on our understanding of pollutant assimilation processes, as well as depuration/egestion rates for aquatic and terrestrial receptors; and
- Limitations on our understanding of population dynamics and seasonal biomass fluctuation for certain receptor species.

Because of the complexity, the current TRIM.FaTE generates enormous amounts of output. There are more than 1,500 links in the TRIM.FaTE prototype in which transition rates are calculated for each time period. Each link contains important information regarding the process being simulated. Proper evaluation of the model requires that the generated information be explored and assessed. This information includes:

- The contribution of various components to the total transition rate (e.g., diffusion versus advection, solid phase advection versus liquid phase advection);
- The contribution of intermediate processes to specific components of the transition rate (e.g., cuticle conductance versus stomatal conductance in calculating diffusion component of the air-to-plant transition rate); and
- The partitioning of the flow of chemical through particular domains.

Limited model verification has been performed to date, but more verification is needed. This may best be accomplished with simple applications that focus on a particular subset of domains.

The driving forces in TRIM.FaTE are the flows of air, water, and solids throughout the system. The modeled chemical(s) will be transported primarily via these mechanisms. While such flows are considered external to the basic structure of the model, rather than part of the model itself, it would be worthwhile to allow the inclusion of additional flow models within the model framework. Numerous models exist for long-term flow (e.g., the Universal Soil Loss Equation for erosion flow), but their application in a dynamic, multi-compartment context must be carefully investigated. Currently, the flow model for air transport is also overly simplistic and other appropriate models or algorithms need to be investigated.

6.5 Conclusions from Developmental Work on TRIM and TRIM.FaTE

Detailed single-media models, such as Gaussian-plume models, subsurface transport models, and surface water models, exist for a variety of applications. Some multimedia models are based on the linking of these detailed

single media models; MEPAS is one example⁴⁵. However, it is extremely difficult to impose strict mass balance relationships, implement thermodynamics of partition processes, and carry out comprehensive sensitivity and uncertainty analyses with these “linked-model” systems¹⁵. In contrast, the Mackay-type multimedia models provide strict mass balance relationship, use fugacity capacities (that is the capacity of a compartment to contain a chemical on a unit volume-basis) to define the kinetics and limits of mass transfer, and provide a tractable and scientifically defensible framework for assessing pollutant behavior in complex systems^{17,31}.

TRIM.FaTE was designed to fill the middle ground between the more spatially complex single-media models and the comprehensive but often low-resolution multimedia mass-balance models. TRIM.FaTE is a Mackay-type multimedia model based on the following criteria: it uses a series of fully interacting compartments to represent all components of an environmental system; and it is fully mass-balancing, and uses fugacity-based relationships to define the kinetics and limitations of mass transfer processes.

However, unlike any Mackay-type multimedia model to date (for examples see *The Multimedia Fate Model: A Vital Tool for Reducing the Fate of Chemicals*³¹), TRIM.FaTE is designed to accommodate relatively short time steps and high spatial resolution. In addition, unlike most multimedia models, TRIM.FaTE has the capability of simulating non-reversible liquid-solid sorption processes in soil and of simulating the coupled transport and transformation of multiple chemical species.

TRIM.FaTE currently has a spreadsheet interface with compiled FORTRAN modules used as equation-solving routines. This arrangement facilitates sensitivity and uncertainty analyses and makes possible the analysis of alternate algorithms for linking compartments.

6.5.1 Prototype Algorithms and Mathematical Structure

Tests of a prototype version of TRIM.FaTE indicate that the multimedia approach produces realistic mass distributions in ecosystems containing representative air, water, soil, plant, and animal compartments.

TRIM uses a dynamic mass-balance approach to provide estimates of the exposure and dose profile received by selected receptors. The TRIM.FaTE module accounts for the movement of pollutant mass through a user-defined, bounded systems model that includes both biotic and nonbiotic (abiotic) compartments. The compartments have index addresses that represent the spatial location, domain type, and chemical species of the pollutant. The model uses mass balance relationships, fugacity capacities, and biokinetics to determine the movement of pollutant mass among the compartments. A system of linked differential equations describing pollutant mass transfer rates between pairs of addresses is at the heart of this model.

The features that make the mathematical structure of TRIM.FaTE (Chapter 3.0) unique are: (1) its system of linked differential equations across all locations, environmental domains, and chemical species; and (2) the estimation of transfer factors between cells based on a library of algorithms. These features provide flexibility in defining the complexity of a simulation.

6.5.2 *Input Data Needs, Verification, and Validation*

Data sets needed to carry out TRIM.FaTE assessments include: chemical properties data, including basic chemical properties and transformation rates; landscape data, including ecosystem, land use, hydrology, and climate data; and nonchemical-specific biotic parameters. TRIM.FaTE concentration estimates are to be as spatially and temporally explicit as is feasible. The data needed for the spatial explicitness of TRIM.FaTE will be provided by a GIS containing readily available national or regional data sets for required model parameters such as land cover, soil characteristics, roads, water bodies, presence and abundance of species or biomass, and climate variables. A default set of spatial data for biotic and abiotic parameters has been identified.

7.0 Summary, Discussion, and Future Directions

The OAQPS has the regulatory responsibility for hazardous and criteria air pollutant programs under the CAA. A broad range of risk assessments are needed to support regulatory decision making for these programs. The OAQPS has embarked on a 4-year effort to develop a total risk modeling system, and the components of that system, for use in assessing human health and ecological risk and exposure in support of HAP and criteria pollutant programs under the CAA. TRIM will provide a framework for assessing human health and ecological risks resulting from multimedia, multipathway exposure to HAPs and criteria pollutants. The goal is to develop a framework that is scientifically defensible, flexible, and user-friendly, and that meets the broad range of risk assessments required under the various CAA programs and supports regulatory decision-making for these programs. This section discusses the progress made to date on the development of TRIM, the limitations and uncertainties identified with respect to TRIM, and plans for future development.

7.1 Progress to Date

Progress on TRIM, to date, has been in two main areas: (1) the definition of TRIM, including the overall conceptual design and detailed plans for development; and (2) the development of a prototype of TRIM.FaTE, the first module within TRIM (Figure 2-1).

7.1.1 Conceptual Design of TRIM: Design Goals and Objectives

TRIM is intended to be the next generation of environmental risk and exposure models for OAQPS. Developing a predictive environmental model of chemical transfers to human and ecological endpoints that is flexible and applicable to both criteria pollutants and HAPs, while incorporating multimedia, multipathway exposures, is a complex problem. To be successful, TRIM must address the range of spatial and temporal scales, endpoints, and pathways of interest to specific CAA programs. TRIM is expected to be a very complex model that can depict a range of environmental and physical processes. Balance is needed in the design of the model. One of the most critical mistakes a system developer can make is to create a system that is too complex. Therefore, clarity must be maintained on what model processes and outputs are really needed, how those outputs are going to be used, and how precise they need to be. A quality systems approach demands that the endpoints be considered carefully and analyzed rigorously at the beginning of a project so that the planning and design will satisfy the true project objectives. As a result, efforts have been made to clearly establish the overall objectives of TRIM and to identify specific design features that can be used to measure progress and performance of both the overall modeling system and its individual components.

TRIM consists of six individual modules (see Chapter 2.0), each addressing a major element affecting risks associated with environmental pollutants. These six components allow for a phased approach for development.

These six modules are intended to address specific processes affecting environmental fate and transport, exposure, and dose (absorbed and target organ). It should be noted that there is no clear delineation between the modules. Actual boundaries may be blurred between the components for specific applications. For example, TRIM.FaTE is intended to estimate pollutant concentrations in various environmental compartments that serve to define, temporally, exposures for individuals as they move through the modeled area over time. However, TRIM.FaTE essentially is a complete model for stationary ecological receptors (e.g., worms), incorporating exposure and uptake for these receptors. Exposure of mobile ecological receptors to contaminants may be modeled by also using the Exposure Event Module.

Furthermore, the use of six modules allows for flexibility in both the development and application of TRIM. Modules can be developed in a phased approach as science permits while using standard default parameters and algorithms until more detailed information becomes available. For example, standard assumptions regarding pollutant uptake can be used until a model is developed or chemical-specific data become available. The development of TRIM.FaTE, a prototype environmental fate, transport, and exposure model, demonstrates the practicality of both phased development and flexible modular design. Specific details of how future modules will be developed and how they will be integrated are still under development.

7.1.2 TRIM.FaTE Module Development

TRIM.FaTE demonstrates the practicality of a phased modular development, which allows integration of the most current scientific advances. How TRIM.FaTE meets the major design goals for TRIM of scientific defensibility and flexibility are discussed throughout the report and are summarized in the following paragraphs.

- **Scientific Defensibility.** TRIM.FaTE (discussed in detail in Chapters 3.0 through 5.0) represents an innovative model that addresses many of the concerns with previous multimedia models. TRIM.FaTE is a true coupled multimedia model rather than a linked model system. As a result, it is truly mass conserving and allows for the estimation of both spatial and time-step analyses, thereby allowing for non-equilibrium analysis. The case study using two organic pollutants has demonstrated the model's flexibility in addressing the fate and transport of multiple pollutants. In general, TRIM.FaTE was developed in an iterative manner through a series of phases where the model complexity was increased with each project phase.
- **Flexibility.** TRIM.FaTE has demonstrated flexibility in its modular nature, spatial and temporal resolution. Its ability to assess both human and ecological risks will be further demonstrated by the other TRIM modules. In addition, TRIM.FaTE estimates time series concentrations in various environmental media, which would allow for moving (human or ecological) receptors through these components and allow for estimating exposure and concomitant risk to human and ecological receptors. As previously stated, prototypes can be used individually to support analysis of varying levels of complexity. Another major feature of TRIM.FaTE is the algorithm library, which allows for flexibility by readily

integrating future data or scientific advances into the model as they become available.

TRIM.FaTE also appears to provide the basic foundation to support analysis in subsequent modules. By estimating pollutant mass distributions as a function of time and space in various environmental domains, the foundation is laid for moving human and ecological receptors in time and space through these domains to estimate exposure. The ability to address seasonal and other temporal dimensions of these movements also exists. Therefore, TRIM.FaTE integrates well with the latter TRIM modules, specifically the Exposure Event Module.

7.2 Limitations and Sensitivity

One of the greatest concerns in developing TRIM's individual modules is the complexity of the model. Complexity of the model is of concern because it leads to: excessive computation, due to its mathematical structure; burdensome data needs; and requirement of a sophisticated user.

A multimedia model describing the world in true detail would be highly complex. It is unlikely that a model could be developed to simulate the real world. Whether all processes are defined is not known, and to account for all processes would be an ambitious undertaking. Obscure and seemingly unimportant relationships may actually provide some critical feedback mechanism and, if not accounted for, may result in errors in long-term projections. Attempting to include a broad range of mathematical relationships increases the potential for inconsistencies between parameters that may not have mathematical solutions. Furthermore, with complex modeled systems, there is a magnified importance in initialization settings for the model. With complex systems, minor differences in initialization settings can lead to vast differences in final modeled estimates. The lack of well-defined initialization settings (e.g., due to lack of data, definition of background) is to be expected for any setting to be modeled and, therefore, may be a problem in TRIM if the model is too complex. The sensitivity of the model to these effects will continue to be addressed in future model evaluations.

Complex models include a multitude of parameters. The value of such models is dependent on the quality and quantity of data for each parameter. The model may only be as good as the lowest quality data available for an individual parameter. Also, given the large number of parameters, large quantities of data may be needed to run the model. TRIM.FaTE represents only one component of TRIM and the test case application has shown the need for large data sets. The developers of TRIM have focused attention on developing a model that is dependent on basic physical and chemical properties of pollutants. These data are generally available in the literature, if somewhat uncertain. However, there are numerous other data needed, some of which may be difficult to obtain on the temporal and spatial scales required for site-specific assessments. The success of TRIM.FaTE, future TRIM components, and the overall approach is dependent on obtaining critical parameters and furnishing these data in a readily accessible database. Requiring the user to collect voluminous data for every new application may prohibit TRIM.FaTE usability. However, it is unlikely that a library of default data

distributions can be developed that would be appropriate for all applications.

Multimedia risk assessment models by nature are very complex and draw on a broad range of disciplines (e.g., from meteorology to plant physiology in TRIM.FaTE). It is unreasonable that any one individual has a fundamental understanding of all parameters and relationships contained in the model. Therefore, the goal of TRIM is to develop a system that minimizes the detail to which a user would be required to make judgements. To this end, the model and possible structures must be fully evaluated to determine the appropriate detailed relationships and the user would be required only to establish general relationships. Well-studied generic settings may also prove useful. The model must be designed to prevent the user from proposing invalid relationships or scenarios. Therefore, a detailed evaluation of the TRIM.FaTE (and future modules) structure, uncertainty, and sensitivity is essential to determine the appropriate model structure and level of user defined options. For example, TRIM.FaTE could be designed to allow the user to be responsible for defining all linkages, or could be set up to develop detailed linkages based on generic relationships defined by the user.

One of the key limitations in multimedia models is the lack of model validation opportunities. Ideally, detailed environmental compartment monitoring data would be available for comparing model results to monitoring data. However, very limited data exist in a detailed enough manner to allow for evaluating environmental concentrations specific to a single modeled source on regional scales. As a result, model-to-model comparisons are the best validation processes available, although the magnitude of how they describe reality is not fully known. Comparisons of TRIM.FaTE to other modules is further complicated by the fact that it is a truly coupled multimedia modeling system. TRIM.FaTE has been shown to describe processes of pollutant movement that appear reasonable based on the understanding of environmental systems (i.e., the re-emission from water and deposition on the forested land).

Current model development has focused on site specific applications or generic settings. A detailed analysis has not been made that evaluates the contribution of site-specific data to the overall variability and uncertainty of risk estimates. If site-specific data can be shown to be a small relative contributor to overall uncertainty as compared to more ubiquitous parameters, the use of generic environmental settings may be feasible. Generic settings would minimize the need for user input and judgement. Regardless of whether this is the case, there may also be the question of establishing initialization (baseline) settings for any model application.

The uncertainties and limitations associated with TRIM.FaTE may apply to other also specific modules (e.g., data, mathematic complexity, user sophistication). There may be other overall limitations that are applicable to TRIM. Future modules of TRIM may not be supported by current science and their development may have to be in stages. For example, physiologically-based pharmacokinetic (PBPK) models are currently being developed and validated on a chemical-specific basis. Whether current science allows for generic PBPK models is not known. Likewise, the dose-response module is limited by current agency policy and guidance for evaluating risk

to noncarcinogens, focusing on a threshold hazard quotient approach as opposed to true dose-response. Therefore, progress may be limited on several of the future modules. However, it should be noted that these limitations or delays may only be in the near future, and that the design of TRIM (i.e., modular design) allows for readily integrating the most current science as it becomes available.

Given the complexity and limitations of multimedia modeling, some questions have been raised regarding applicability of multimedia risk assessment results. The Science Advisory Board (SAB), in their review of the Mercury Report to Congress⁴⁶, has stipulated that, given the uncertainties associated with such multimedia models, their accuracy is questionable and, therefore, can only be used as a qualitative comparative measure of risk and not for quantitative purposes. Therefore, until TRIM can be validated and detailed sensitivity and uncertainty analysis be conducted, its usefulness will most likely be limited to qualitative analyses.

7.3 Future Development

TRIM is intended to be developed in a phased approach. A total of six modules have been identified for development. Once these are completed, risk assessments can be conducted in a comprehensive manner. However, default assumptions or scenarios can be used in their place until all modules are completed. As a result, the usefulness of TRIM is not contingent upon completion of all modules. Each module only increases the overall confidence of the risk estimates and allows for evaluating variability and uncertainty in greater detail. For example, if uptake and biokinetic models are not available, concentration response relationships could be used to support the risk assessment.

7.3.1 Overall TRIM Development

To maximize the usefulness of TRIM, the phased approach will be emphasized, and the focus of these efforts will be module development and platform integration. Modules will be developed according to their perceived overall importance and the current status of applicable science. In addition, to facilitate the integration of individual modules, computer platforms will be evaluated to determine which is most appropriate for addressing the existing modules and for directing future module development. The schedule proposed for further TRIM module development and release of TRIM is as follows:

Fiscal year (FY) 1998:	SAB review of TRIM approach and TRIM.FaTE TRIM.FaTE refinement (see Section 6.6) Exposure event model prototype TRIM computer framework design
FY 1999:	SAB review of exposure event model Risk characterization module prototype Other TRIM modules
FY 2000 and beyond:	TRIM beta testing.

Release of TRIM for public use.

TRIM was intended as a 4-year effort. It is unlikely that the complete TRIM modeling system, as conceptualized, will be completed in that time frame. Rather, efforts will focus on maximizing the utility of the overall modeling system. It is anticipated that refinement of the TRIM.FaTE module will be completed, together with prototypes for the exposure-event model and risk characterization model by FY 1999. It is anticipated that these prototypes will be evaluated and improved, and that a complete TRIM prototype will be available for beta testing in FY 2000.

7.3.2 TRIM.FaTE Development

TRIM.FaTE currently consists of multiple prototypes under refinement. Development continues to focus on refinement of TRIM.FaTE and features development of a version programmed in optimized computer language and in a form that can be easily used and widely distributed. Future development and testing of TRIM.FaTE will be focused on four main areas:

- Expansion of ecological algorithms and features
- Uncertainty and sensitivity analysis
- Model verification and validation
- Database development.

Expansion of Ecological Algorithms and Features. One of the key areas of emphasis in the future development of TRIM.FaTE will be improvement of the ecological links in the model. Several new algorithms will be added to the model, and the parameterization of existing algorithms for ecological receptors will be improved. Additional algorithms will be required for many chemical transfers to allow the fate of inorganic chemicals to be modeled.

Distributions or ranges of several wildlife parameters will be added to the database for TRIM.FaTE, including ingestion and inhalation rates, elimination rate constants (or half-lives) for particular chemicals, and population densities for particular ecosystems. Data contributing to distributions of lipid levels in fish will be collected. Algorithms for chemical transfers to fish and benthic organisms will be parameterized for additional representative species. The creation of new wildlife domains will not be a priority in the near-term; representative species have been selected for all major food-web groups.

Domains for seeds and fruits (and perhaps wood and bark) will be created, and all plant cells will be linked. A domain for algae will be created. Adjustments of algorithms and parameters based on plant taxa (e.g., waxy versus non-waxy leaves) will be considered. Spatial data sets for parameters such as leaf-area index and vegetation biomass will be obtained.

Seasonal processes, such as litterfall, plant growth and senescence, crop harvesting, migration of wildlife, wildlife food habits, and winter sleep will be incorporated into TRIM.FaTE, to the extent possible. Other changes in biomass, such as organism and population growth and death, will be incorporated into the model, either through growth functions or through changes in monthly biomass input parameters. The movement and reproduction of wildlife and fish must be represented in a simplified manner, since individual-based models for many species would not be feasible.

Model outputs will be compared to empirical data, to the extent possible. Assumptions will be based on the best available science. At this time, for example, it is clear that the masses of contaminants estimated in wildlife, earthworms, and plant roots are very sensitive to the choices of the soil depth interval from which incidental ingestion or accumulation of chemicals in soil occurs.

Significant effort will be focused on estimating uncertainty bounds for all half-life terms, both in biota and abiotic media.

7.3.3 Exposure Event Module

Work on the Exposure Event Module is ongoing. This module will be used to translate pollutant sources (indoor and outdoor) into quantitative estimates of the amount of contaminant that comes in contact with the human-environment boundaries, that is, the lungs, the GI tract, and the skin surface of individuals within a specified population. Human exposures within TRIM.FaTE will be modeled through the use of “cohort” models within reference indoor/outdoor environments. Each cohort will consist of a group of persons with similar physical and demographic characteristics who follow a common activity pattern. The activity pattern of each cohort will consist of a realistic, time-ordered series of exposure events. Each exposure event will be defined by a start time, an end time, and a list of compartments in the study area to which the cohort is exposed during the event (e.g., air and soil associated with the indoor domain). An uptake equation specific to each compartment in the list is applied to the current pollutant concentration of the compartment to determine the potential dose received by the cohort. The total dose received during the exposure event is the sum of the doses received from the individual compartments.

7.3.4 Development of Uncertainty and Sensitivity Analysis Capabilities

An important component of the TRIM program in the next 2 years will be to focus on uncertainty and sensitivity analyses. Initially, focus will be on parameter uncertainty. As previously discussed, each model input can be entered as a distribution such that Monte Carlo simulations can be completed to examine the range of possible outputs. Although parameters can be entered as distributions at this time, the methods for constructing and entering parameter distributions need to be optimized such that Monte Carlo simulations can be processed more efficiently.

Methods for conducting and evaluating model uncertainty analysis need to be better defined, carried out, and evaluated. The current approach is to select among alternative algorithms from the algorithm library for each transport and transformation process. By looking at the change in resulting output, the effects of model uncertainty and the influence of each process can be evaluated. Although this can be done manually in the TRIM framework, a system to automate this process needs to be developed.

The system to evaluate spatial and temporal variability needs to be automated. Changing the spatial step size or temporal step size can change the results of the model. Evaluating the effect of this change helps the researcher decide what scale is appropriate for their needs.

Ultimately, TRIM will provide a framework that facilitates probabilistic analyses, including the use of correlation, rank correlation, or regression to examine the degree to which outcome variance is attributable to particular inputs or assumptions, and helping the user to better focus data gathering efforts. Additionally, completing an uncertainty analysis facilitates the comparison of model predictions to limited multimedia environmental data. Implementing output ranges and parameter uncertainty dependence will help the model validation stage of TRIM.FaTE.

8.0 References

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APPENDIX A

GLOSSARY

Glossary

Advection - Process in which a chemical is transported within a given moving phase that is moving from one cell to another. Calculation of advective flux requires velocity of and amount of chemical in the moving phase. MacKay 1991 refers to advection as the “piggyback” process, in which a chemical “piggybacking” on material moving from one place to another for reasons unrelated to the presence of the chemical.

Atmospheric Half-Life - The time required for one-half of the quantity of an air pollutant to react and/or break down in the atmosphere.

Bioaccumulation - Progressive increase in amount of chemical in an organism or part of an organism that occurs because the rate of intake exceeds the organism’s ability to remove the substance from the body.

Bioconcentration - Same as bioaccumulation; refers to the increase in concentration of a chemical in an organism.

Biological Half-Life - The time required for the concentration of a chemical present in the body or in a particular body compartment to decrease by one-half through biological processes such as metabolism and excretion.

Carcinogenic - Able to produce malignant tumor growth. Operationally, most benign tumors are usually included also.

Cell - A uniquely defined address, within the computer code, which accounts for all potential locations of mass within the ecosystem. The three indices that make up an inventory address in TRIM.FaTE are volume element, domain, and species. There is no concentration gradient within an inventory address; the chemical is uniformly mixed. Also referred to as inventory address.

Clean Air Act of 1990 - This amendment to the Clean Air Act of 1970 contains several provisions requiring the EPA to evaluate effects to humans and the environment caused by exposure to hazardous air pollutants and criteria air pollutants.

Cohort Study - A study of a group of persons sharing a common experience (e.g., exposure to a substance) within a defined time period: this experiment is used to determine if an increased risk of a health effect (disease) is associated with that exposure.

Compartmental Systems Model - A model that is represented by a series of inventory addresses, each with a state variable, which interact through transfer factors. In this model, the transport of multiple pollutant species in a multimedia region is set up as a mass exchange among a set of systems used to represent spatial locations, collections of environmental phases, and chemical species.

Criteria Pollutant - Six common pollutants, used as indicators of air quality, regulated by EPA on the basis of human and/or environmental adverse effects.

Dermal Uptake - Absorption through the skin membrane.

Diffusion - Movement of a chemical substance from areas of high concentration to areas of low concentration. Biologically, diffusion is an important means for toxicant deposition for gases and very small particles in the pulmonary region of the lungs.

Dispersion Model - A mathematical model or computer simulation used to predict the movement of airborne pollution. Models take into account a variety of mixing mechanisms which dilute effluents and transport them away from the point of emission.

Domain - The domain refers to the composition of material in which the chemical is dissolved, sorbed, or otherwise held. What distinguishes one domain from another at a given location is the requirement that all phases of a single domain must attain equilibrium within a single calculation time step. There is a hierarchical system of domain, i.e., different levels of domain. At a more general level, a domain is a collection of volume elements, such as all of the root zone soil. For example, an instance of the domain is the root zone soil within a volume element.

Dose - The amount of chemical absorbed by an organism usually expressed as mass of substance per unit body weight of organism per unit time.

Dose Response - Determination of the magnitude of toxic response to dose.

Dry Deposition - A transfer process from air to soil. Dry deposition velocity is the ratio of contaminant flux ($\text{mol}/[\text{m}^2\text{-h}]$) to contaminant concentration in air (mol/m^3).

Environmental Fate - The destiny of a chemical or biological pollutant after release into the environment. Environmental fate involves temporal and spatial considerations of transport, transfer, storage, and transformation.

Equilibrium - The state in which opposing forces are exactly counteracted or balanced. Types of equilibrium include acid-base, colloid, dynamic, homeostatic, and chemical. Used in risk assessment of toxic air pollutants to generally describe the chemical equilibrium between a pollutant in the inhaled air and the level in the body.

Exposure Assessment - Measurement or estimation of the magnitude, frequency, duration and route of exposure of animals or ecological components to substances in the environment. The exposure assessment also describes the nature of exposure and the size and nature of the exposed populations, and is one of four steps in risk assessment.

Hazardous Air Pollutant - Any air pollutant listed pursuant to Section 112(b) of the Clean Air Act of 1990. Those pollutants known or suspected to cause serious health problems.

Half-Life - See atmospheric half-life and biological half-life. Also, the period of time characteristic of a radionuclide in which one-half of the activity has decayed.

Indices - There are three indices used in the inventory address and state variable used as a tracking and auditing system to clarify the volume element, domain, and species in the TRIM.FaTE framework.

Indirect Exposure Methodology - This methodology sets out procedures for estimating the indirect (i.e., non-inhalation) human exposures and health risks that can result from the transfer of emitted pollutants to soil, vegetation, and water bodies. This methodology is not a comprehensive environmental audit, but is best regarded as an evolving and emerging process that moves the EPA beyond the analysis of potential effects on only one medium (air) and exposure pathway (inhalation) to the consideration of other media and exposure pathways.

Ingestion Uptake - Intake via the mouth, with transfer to the GI tract.

Inhalation Uptake - Intake via the nose and mouth, with transfer to the lungs

Inventory Address - A uniquely defined address, within the computer code, which accounts for all potential locations of mass within the ecosystem. The three indices that make up an inventory address in TRIM.FaTE are volume element, domain, and species. There is no concentration gradient within an inventory address; the chemical is uniformly mixed. An informal synonym for this term is “cell.”

Links - If mass moves without first moving through intervening cells, the two cells are considered linked. Each linkage is associated with an algorithm determining the direction and rate of mass flow between the two cells.

Multi-Pathway Exposure - Exposure through inhalation, ingestion, and adsorption routes.

Microenvironment - The immediate local environment of an organism.

Model - A mathematical representation of a natural system intended to mimic the behavior of the real system, allowing description of empirical data, and predictions about untested states of the system.

Models-3 - EPA's third generation of air quality management/modeling system to be used as a tool for decision making by federal, state and the industry environmental analysts. It is a layered modeling system providing various kinds of services at various levels of complexity. The most important layers are the User, Management, Computational Modeling, and Data Access layers.

Multimedia Contamination - Contamination in air, water, soil, and food.

Pharmacokinetics - The field of study concerned with defining, through measurement or modeling, the absorption, distribution, metabolism, and excretion of drugs or chemicals in a biological system as a function of time.

Phase - The building blocks of which everything else is composed (gas, liquid, solid, lipid, and other material). Each **domain** consists of multiple phases.

Reaction or "R" Factor - Used for chemical reactions or transformation processes. Used for transfer from one species to another (e.g., radioactive decay), or for transfers out of the system (e.g., chemical degradation to a chemical not being tracked). As an example, consider an address that represents a soil layer contaminated with trichloroethylene (TCE). This address will be at the same location and represent the same domain, but differs in the last entry from the address that represents the inventory of vinyl chloride (VC), which is a decay product of TCE. Both addresses are at the same location and domain, but TCE must undergo a transformation to move from the address with the TCE/soil layer to the VC/soil layer address.

Reaction Transformation - Process that transforms a chemical species into another chemical species, but does not include a change of location or domain. Biodegradation, photolysis, hydrolysis, oxidation/reduction, radioactive decay, etc., are reaction transformation processes.

Risk Assessment - The scientific activity of evaluating the toxic properties of a chemical and the conditions of human exposure to it in order both to ascertain the likelihood that exposed humans will be adversely affected, and to characterize the nature of the effects they may experience. May contain some or all of the following four steps:

Hazard Identification - The determination of whether a particular chemical is or is not causally linked to particular health effect(s).

Dose-Response Assessment - The determination of the relation between the magnitude of exposure and the probability of occurrence of the health effects in question.

Exposure Assessment - The determination of the extent of human exposure.

Risk Characterization - The description of the nature and often the magnitude of human risk, including attendant uncertainty.

Risk Characterization - The final step of a risk assessment, which is a description of the nature and often the magnitude of human risk, including attendant uncertainty.

Risk Management - The decision-making process that uses the results of risk assessment to produce a decision about environmental action. Risk management includes consideration of technical, scientific, social, economic, and political information.

Sink - A domain that receives input from a domain, but does not output the chemical. Once a chemical enters a sink, its mass is not tracked in the model; it is a final “resting place” for the chemical.

Species - Chemical compound state/phase (i.e., form of the chemical and phase of the chemical-physical properties of the chemical) This index is useful for representing radioactive decay or chemical decay, (e.g., TCE to vinyl chloride).

State Variable - Values that describe the state of the system as a function of time in the various components of the modeled system.

Transfer Factors - The rate at which a chemical will be transferred from one inventory address to another inventory address for a given mass in that inventory address. The units of this factor are fraction of total

inventory per unit time. When a transfer rate factor is multiplied by an inventory expressed as mass, we obtain from this product the mass transferred per unit time. There are three types of transfer factors, “T” factor and “R” factor, for transport, reaction, and exchange, respectively. It should be noted that the magnitude of transfer rates do not define the magnitude of the transfer because if there is very little mass in a cell, there will be very little transferred.

Transformation - Alteration of a chemical substance from one chemical form to another through a chemical, physical, or biological reaction.

Transport or “T” Factor - This transfer rate can be used in several ways. First, it can be used for **transport** from one location to another. This is further broken down into transport processes involving the change of location by advection or by diffusion. At a minimum, there will be a change in the first index, the spatial location for this type of process, i.e., diffusion in the soil. Sometimes, there will be both a change of domain and spatial location, i.e., diffusion from air to soil. An alternate use is for transfer from one domain to another at the same spatial location, in which case the second index changes. For example, if we decide that sediment particles should not be in equilibrium with water, then the water and the particles would have to be separate domains at the same volume element and a “**T**” **factor** would be used to express the exchange between these phases.

Transport - To move or be conveyed from one place to another. In the context of environmental contamination, a containment is transported from one location to another by dispersion, advection (e.g., wind), or diffusion (e.g., dilution in air) processes.

Volume Element - An entity characterized by a total spatial volume (m^3) completely enclosed by a contiguous surface. This surface may be shared by one or more neighboring volume elements. The volume element has a unique spatial location, which can be defined with a set of x-y-z coordinates. The volume is occupied by all **domains** at this location. For example, if there are two **domains** at a **volume element**, the sum of the volumes of these two **domains** must sum to the volume of the **volume element**. When two domains occupy the same volume location, these two domains are assumed to be well mixed.

Wet Deposition - Transfer process from air to soil. Occurs during precipitation and is proportional to the rate of precipitation (i.e., rain in m/h), but differs in both the relative magnitude and nature between particles and gas-phase chemicals.

APPENDIX B

ALGORITHM GENERALIZATIONS

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ALGORITHM GENERALIZATIONS

One of the goals of the TRIM modeling framework is to develop underlying generalizations, estimation techniques or “rules”, for application of algorithms. During the development of the transfer factors for the prototypes, common rules were observed. These rules were functions of the physics and chemistry of the transport processes rather than the domains. For example, abiotic transport from one cell to another has the same mathematical form for all domains. Some of these rules were refined after study of their documentation in the literature (McKone, 1996, MacKay, 1992). This appendix documents the underlying rules for use in subsequent prototypes in order to simplify algorithm development. These rules were observed as a consequence of building the transfer factors for the different abiotic domains and are presented before the domain specific algorithms because the rules are common across all the abiotic domains.

B.1 Multiple Phase Calculations

This section describes how multiple phases within a domain are modeled in P4. Phases considered in P4 are liquid, gas, and solid and are assumed to be at chemical equilibrium. Because chemical equilibrium is assumed, the ratios of the concentrations in the individual phases are constant, and mass balance need only be tracked for the total amount of the chemical in all phases in a cell. The amount of chemical in the cell in a particular phase can be determined from the total amount in the cell (this is described below). It is possible that, in later prototypes, chemical equilibrium will not be assumed, in which case the amount of chemical in different phases will need to be tracked as separate cells.

In any cell, the total amount of chemical in a given cell is made up of the sum of the amounts in the different phases:

$$\begin{aligned} N_i^{Total} &= \text{Amount in gas phase} + \text{Amount in aqueous phase} + \text{Amount in solid phase} \\ &= C_i^{gas} V_i^{gas} + C_i^{water} V_i^{water} + C_i^{solid} V_i^{solid} \end{aligned}$$

where:

$$\begin{aligned} N_i^{Total} &= \text{total amount of chemical in domain/cell, units of } g [\text{chemical}] \\ C_i^{gas} &= \text{concentration of chemical in gas phase in domain/cell, units of } g [\text{chemical}] / m^3 [\text{gas}] \\ &\quad \text{in domain} \\ V_i^{gas} &= \text{volume of gas in domain/cell, units of } m^3 [\text{gas}] \text{ in domain} \end{aligned}$$

$$C_i^{water} = \text{concentration of chemical in aqueous phase in domain/cell, units of } g [chemical]/m^3[water] \text{ in domain}$$

$$V_i^{water} = \text{volume of aqueous matter in domain/cell, units of } volume [aqueous] \text{ in domain}$$

$$C_i^{solid} = \text{concentration of chemical in solid phase in domain/cell, units of } g [chemical]/m^3[solid] \text{ in domain}$$

$$V_i^{solid} = \text{volume of solid in domain/cell, units of } m^3[solid] \text{ in domain}$$

If it is desired that the units of N_i^{Total} be in units of *moles [chemical]*, then the preceding equation must be multiplied by the molecular weight of the chemical (which has units of *moles chemical/g [chemical]*)

Since chemical equilibrium is assumed, the ratios of the concentrations are constant. However, care must be used in specifying what the units of the concentrations are. This is because, in practice, it is more common to define notation for ratios of concentrations on a mass basis other than that of mass by volume basis.

B.1.1 Normalization to Liquid Phase

This section describes the relevant formulas when the concentrations are normalized to the concentration in the liquid phase. This normalization is utilized in P4 for all soil, surface water, and sediment cells. Using the equilibrium assumptions, we have that:

$$C_i^{solid} = (\rho_{solid} K_d C_f) C_i^{water}$$

$$C_i^{gas} = (H/RT) C_i^{water}$$

where:

$$\rho_{solid} = \text{density of solid phase in cell, units of } kg[solid \text{ phase}]/m^3[solid \text{ phase}]$$

$$K_d = \text{equilibrium partition coefficient; ratio of concentration in solid phase (units of } kg[chemical]/kg[solid \text{ phase}]) \text{ to that in liquid phase (units of } kg[chemical]/Liters[liquid \text{ phase}])$$

$$C_f = 10^{-3} m^3/L, \text{ conversion factor to convert } m^3 [liquid \text{ phase}] \text{ to } Liters[liquid \text{ phase}]$$

$$H = \text{Henry's law constant for chemical, units of } Pa \cdot m^3/mol$$

$$R = \text{ideal gas constant, } 8.314 m^3 \cdot Pa/mol \cdot K$$

$$T = \text{temperature, units of degrees } K$$

Applying these relationships to the general equation in the beginning of this section yields:

$$N_i^{Total} = C_i^{water} \left(\frac{H}{RT} V_i^{gas} + V_i^{water} + \rho_{solid} K_d C_f V_i^{solid} \right)$$

The volumes of each phase in the domain can be expressed as fractions of the total volume of the cell, in which case the above equation yields:

$$N_i^{Total} = C_i^{water} V_i^{Total} \left(\frac{H}{RT} \frac{V_i^{gas}}{V_i^{Total}} + \frac{V_i^{water}}{V_i^{Total}} + \rho_{solid} K_d C_f \frac{V_i^{solid}}{V_i^{Total}} \right)$$

where:

$$V_i^{Total} = V_i^{gas} + V_i^{water} + V_i^{solid}$$

The term $C_i^{Total} = N_i^{Total} / V_i^{Total}$ is the total concentration of the chemical in the cell. Using the assumed equilibrium relationships, the concentrations in the individual phases can be recovered from the total amount of mass in the cell, as follows:

$$C_i^{water} = \frac{N_i^{Total} / V_i^{Total}}{\left(\frac{H}{RT} \frac{V_i^{gas}}{V_i^{Total}} + \frac{V_i^{water}}{V_i^{Total}} + \rho_{solid} K_d C_f \frac{V_i^{solid}}{V_i^{Total}} \right)}$$

$$C_i^{gas} = \frac{H}{RT} C_i^{water} = \frac{(H/RT) N_i^{Total} / V_i^{Total}}{\left(\frac{H}{RT} \frac{V_i^{gas}}{V_i^{Total}} + \frac{V_i^{water}}{V_i^{Total}} + \rho_{solid} K_d C_f \frac{V_i^{solid}}{V_i^{Total}} \right)}$$

$$C_i^{solid} = \rho_{solid} K_d C_f C_i^{water} = \frac{(\rho_{solid} K_d C_f) N_i^{Total} / V_i^{Total}}{\left(\frac{H}{RT} \frac{V_i^{gas}}{V_i^{Total}} + \frac{V_i^{water}}{V_i^{Total}} + \rho_{solid} K_d C_f \frac{V_i^{solid}}{V_i^{Total}} \right)}$$

For cases in which the concentration in the water phase is negligible (e.g., when domain is the atmosphere, or the chemical has a very low solubility), the concentrations must be normalized to another phase.

The preceding equation can be simplified by using the notation of fugacity. The fugacity capacities for the pure phases are defined by Mackey, 1991.

$$Z_{water} = 1/H$$

$$Z_{air} = 1/(R T)$$

$$Z_{solid} = \rho_{solid} K_d C_f Z_{water}$$

The total fugacity capacity Z_i^{Total} for the cell is defined as:

$$Z_i^{total} = Z_{air} \frac{V_i^{gas}}{V_i^{Total}} + Z_{water} \frac{V_i^{water}}{V_i^{Total}} + Z_{solid} \frac{V_i^{solid}}{V_i^{Total}}$$

$$\frac{C_i^{phase_1}}{C_i^{phase_2}} = \frac{Z_{phase_1}}{Z_{phase_2}}$$

where *phase* is either the solid, liquid, or gas phase.

Applying these relationships shows that:

$$C_i^{water} = \frac{Z_{water}}{Z_i^{total}} \frac{N_i^{Total}}{V_i^{Total}} = \frac{Z_{water}}{Z_i^{total}} C_i^{total}$$

$$C_i^{gas} = \frac{Z_{air}}{Z_i^{total}} \frac{N_i^{Total}}{V_i^{Total}} = \frac{Z_{air}}{Z_i^{total}} C_i^{total}$$

$$C_i^{solid} = \frac{Z_{solid}}{Z_i^{total}} \frac{N_i^{Total}}{V_i^{Total}} = \frac{Z_{solid}}{Z_i^{total}} C_i^{total}$$

where C_i^{Total} is the total concentration of the chemical in the cell (units of $g [chemical]/m^3[total cell]$). From these relationships, we have that, in general, the amount of mass in the different phases is given by:

$$N_i^{water} = V_i^{water} C_i^{water} = V_i^{water} \frac{Z_{water}}{Z_i^{total}} \frac{N_i^{Total}}{V_i^{Total}} = V_i^{water} \frac{Z_{water}}{Z_i^{total}} \frac{Z_{water}}{Z_i^{total}} C_i^{total}$$

$$N_i^{gas} = C_i^{gas} V_i^{gas} = V_i^{gas} \frac{Z_{air}}{Z_i^{total}} \frac{N_i^{Total}}{V_i^{Total}} = V_i^{gas} \frac{Z_{gas}}{Z_i^{total}} \frac{Z_{gas}}{Z_i^{total}} C_i^{total}$$

$$N_i^{solid} = C_i^{solid} V_i^{solid} = V_i^{solid} \frac{Z_{solid}}{Z_i^{total}} \frac{N_i^{Total}}{V_i^{Total}} = V_i^{solid} \frac{Z_{solid}}{Z_i^{total}} \frac{Z_{solid}}{Z_i^{total}} C_i^{total}$$

where N_i^{water} , N_i^{gas} , and N_i^{solid} are the mass in the water, gas, and solid phases, respectively.

In the following sections, these general equations are applied to the soil and surface water domains. These “applications” involve only adhering to notation commonly used in the literature for the different media.

B.1.2 Application to Soil, Surface Water, and Sediment Domains

For soil, surface water, and sediment domains, the concentrations are normalized to the concentration in the water phase, and the same notation is used to represent the relevant parameters. In a soil cell, the solid phase consists of the soil particles. In a surface water cell, the solid phase consists of the sediment suspended in the water column. In a sediment cell, the solid phase consists of the benthic sediments. Following common practice, the volume fractions of each phase are denoted as follows:

$$\frac{V_i^{water}}{V_i^{total}} = \theta_i$$

$$\frac{V_i^{gas}}{V_i^{total}} = \epsilon_i$$

$$\frac{V_i^{solid}}{V_i^{total}} = 1 - \theta_i - \epsilon_i = 1 - \phi_i$$

where:

$$\begin{aligned} \theta_i &= \text{water} \\ \epsilon_i &= \text{gas} \\ 1 - \theta_i - \epsilon_i &= 1 - \phi_i \end{aligned}$$

where ϕ_i is the total porosity of the cell ($= \theta_i + \epsilon_i$). The equations for the total mass of chemical in the cell and in the different phases are then given by:

$$N_i^{Total} = C_i^{water} V_i^{Total} \left(\frac{H}{RT} \epsilon_i + \theta_i + \rho_{solid} K_d C_f (1 - \phi_i) \right)$$

and the total fugacity for the cell is given by:

$$Z_i^{total} = Z_{air} \epsilon_i + Z_{water} \theta_i + Z_{solid} (1 - \phi_i)$$

For the groundwater, surface water, and sediment domains, the volume fractions of the gas phase (ϵ_i) are assumed to be zero.

In P4, the partition coefficients, soil - water, K_d in each cell (soil, surface water, and sediment) are calculated in a manner applicable for nonionic organic chemicals (Karickhoff 1981, as cited in California Department of Toxic Substance Control's model [CalTOX] 1993, p.25) by:

$$K_d = K_{oc} f_{oc}$$

where:

$$\begin{aligned} K_{oc} &= \text{organic-carbon partition coefficient} \\ f_{oc} &= \text{fraction of organic carbon in the cell/domain} \end{aligned}$$

B.1.3 Multi-Phase Partitioning in the Air Domain

Since the volume of water in an air domain is so small relative to the volume of the solid and the gas phase, there has not been a historical development of K_d 's (i.e., ratio of concentration in solid phase to that in dissolved phase) for the atmosphere, although the concept still applies. Instead, only the solid and gas phases are usually addressed. If chemical equilibrium is assumed between the phases, then a normalization other than to the liquid concentration is required. In an air cell, the solid phase consists of the particulate matter in the atmosphere.

In P4, the volume fractions of chemical in each phase are given by:

$$\frac{V_i}{V_i^{total}} = 0$$

$$\frac{V_i^{solid}}{V_i^{total}} = D_L / \rho_{dust}$$

$$\frac{V_i^{gas}}{V_i^{total}} = 1 - D_L / \rho_{dust}$$

where:

$$D_L = \text{atmospheric dust load in air cell, } kg[aerosol]/m^3[air\ cell]$$

$$\rho_{dust} = \text{density of aerosols, } kg[aerosol]/m^3[aerosol]$$

The dust load and aerosol density are specified in P4. In order to normalize to either the gas or solid phase, the equilibrium ratio of the concentrations in the two phases must be estimated. In P4, the fraction of the contaminant bound to particles, denoted by ϕ_i , is estimated using a method developed in Junge (1977), and is discussed below. Use of this term in the current notation is actually slightly awkward, as:

$$V_i^{solid} C_i^{solid} = \phi_i$$

$$V_i^{gas} C_i^{gas} = 1 - \phi_i$$

From this, the equilibrium ratio of the concentration in the solid phase to that in the gas phase in an air cell is given by:

$$\frac{C_i^{solid}}{C_i^{gas}} = \frac{\phi_i / V_i^{solid}}{(1 - \phi_i) / V_i^{gas}}$$

$$= \frac{\phi_i / (D_L / \rho_{dust})}{(1 - \phi_i) / (1 - D_L / \rho_{dust})}$$

$$= \frac{\phi_i (1 - D_L / \rho_{dust})}{(1 - \phi_i) (D_L / \rho_{dust})}$$

The total mass of chemical in the air cell is then:

$$\begin{aligned}
N_i^{Total} &= C_i^{gas} V_i^{Total} \left((1 - DL_i/\rho_{dust}) + \frac{C_i^{solid}}{C_i^{gas}} (DL_i/\rho_{dust}) \right) \\
&= C_i^{gas} V_i^{Total} \left((1 - DL_i/\rho_{dust}) + \frac{\phi_i(1 - DL_i/\rho_{dust})}{(1 - \phi_i)(DL_i/\rho_{dust})} (DL_i/\rho_{dust}) \right) \\
&= C_i^{gas} V_i^{Total} \left((1 - DL_i/\rho_{dust}) + \frac{\phi_i(1 - DL_i/\rho_{dust})}{(1 - \phi_i)} \right) \\
&= C_i^{gas} V_i^{Total} (1 - DL_i/\rho_{dust}) \left(1 + \frac{\phi_i}{1 - \phi_i} \right)
\end{aligned}$$

The fugacity capacity in the solid phase can be determined by use of the relationship below (see Section 2.1.1).

$$\begin{aligned}
Z_{solid} &= Z_{air} \frac{C_i^{solid}}{C_i^{gas}} \\
&= Z_{air} \frac{\phi_i(1 - DL_i/\rho_{dust})}{(1 - \phi_i)(DL_i/\rho_{dust})}
\end{aligned}$$

The total fugacity in the air cell is then given by:

$$\begin{aligned}
Z_i^{total} &= Z_{air} \frac{V_i^{gas}}{V_i^{Total}} + Z_{solid} \frac{V_i^{solid}}{V_i^{Total}} \\
&= Z_{air} (1 - D_L/\rho_{ust}) + Z_{solid} D_L/\rho_{dust}
\end{aligned}$$

B.1.4 Calculation of the Fraction of Contaminant Bound to Aerosol

In P4, the fraction of contaminant bound to particulate in the air cell, denoted by ϕ_i , is calculated using the method of Junge (1977) as discussed in CalTOX (pp.26-28):

$$\phi_i = \frac{cS}{VP + cS}$$

where:

- VP = vapor pressure or subcooled vapor pressure of the chemical, units of Pa
- c = empirical constant set to 0.173 as in Junge (1977), units of $m\text{-}Pa$
- s = total surface of aerosols per volume of aerosol, units of m^2/m^3 .

There is a range of values for θ , with Whitby (1978) reporting a range of values of $4.2 \times 10^{-5} m^2/m^3$ for a “clean” continental site to $1.1 \times 10^{-5} m^2/m^3$ for urban sites. In P4, the average of these values is used for θ .

Following CalTOX (1993), the subcooled vapor pressure (vapor pressure of subcooled liquid) is used if the temperature is below the melting point of the chemical. In particular:

$$VP = \begin{cases} VP & \text{if } T > T_m \\ \exp[6.79(T_m/T - 1)] & \text{if } T \leq T_m \end{cases}$$

B.2 Converting Equations with Equilibrium Relationships to Dynamic Form

In the course of converting equations to a form that is suitable for use within the intended framework, it is possible to convert some algorithms that represent steady-state equilibrium relationships into time-dependent ones. This can be performed if an estimate of the time required for the concentration to reach some fraction of the steady-state value is available. In particular, if the concentration in one domain/cell C_1 is related to the concentration in another domain/cell C_2 by an equilibrium relationship of the form $C_1 = K C_2$, where K is unknown and it is known that it takes time t_α in order to reach $100\alpha\%$ of the steady-state value when C_2 is approximately constant, then we have that:

$$\frac{dC_1(t)}{dt} = k_2 C_2 - k_1 C_1$$

where k_2 and k_1 are defined below:

$$\begin{aligned} k_2 &= -\ln(1 - \alpha)/t_\alpha \\ k_1 &= K k_2 \end{aligned}$$

Indeed, the solution of the above differential equation with initial condition $C_1(0) = 0$ is given by:

$$C_1(t) = \frac{k_1}{k_2} C_2 (1 - e^{-k_2 t})$$

The steady-state solution is $C_1(t) = (k_1/k_2) C_2$, and so we have that $K = k_1/k_2$. This assumption that $100\alpha\%$ of the steady-state value is reached at time t_α means that:

$$1 - e^{-k_2 t_\alpha} = \alpha$$

Solving for k_2 yields:

$$k_2 = -\ln(1 - \alpha) / t_\alpha$$

When K_2 is determined, $K_1 = K_2$ from which the general result follows.

In P4, this conversion is performed only for the xylem, stem and root cells of the plant domain.

B.3 Advective Processes

An advective process is one in which a chemical is transported within a given phase that is moving from one cell to another (MacKay 1991 refers to this as a *piggyback* process, in which a chemical is “piggybacking” on material that is moving from one place to another for reasons unrelated to the presence of the chemical). All that is required to estimate the advective flux is the velocity of the moving phase, and the amount of the chemical that is in the moving phase. In general, the advective flux in a given phase (e.g., attached to particles, or dissolved in water) from cell i to cell j is given by:

Advective flux from cell i to cell j = (Volume of phase that moves from cell i to cell j per unit time) \times (Amount of chemical in phase per volume of phase in cell i)

or

$$\begin{aligned} \text{Advective flux Cell } i \rightarrow \text{Cell } j &= Q(\text{phase}) \times \frac{N_i(t) \times f_i(\text{phase})}{V_i(\text{phase})} \\ &= T_{i \rightarrow j}^{\text{adv}}(\text{phase}) \times N_i(t) \end{aligned}$$

where:

- $Q(\text{phase})$ = volumetric flux of phase from cell i to cell j , m³[phase]/day
- $N_i(t)$ = amount of chemical in cell i at time t , moles chemical
- $f_i(\text{phase})$ = fraction of chemical in cell i that is in the moving phase, moles chemical in phase/moles chemical in cell i ,
- $V_i(\text{phase})$ = volume of phase that is in cell i , m³[phase],
- $T_{i \rightarrow j}^{\text{adv}}(\text{phase})$ = transition probability for advective flux from cell i to receiving cell, /day, given by:

$$T_{i \rightarrow j}^{adv}(phase) = \frac{Q(phase) \times f_i(phase)}{V_i(phase)}$$

This formula for the transition probability is valid for all advective processes from one cell to another, and does not rely on the fugacity concept. Application of the concept of fugacity shows that (see Section 2.1).

$$f_i(phase) = \frac{Z_i(phase)}{Z_i(Total)} \times \frac{V_i(phase)}{V_i(Total)}$$

where:

$Z_i(phase)$	= fugacity capacity for moving phase, mol/m ³ [phase]-Pa
$Z_i(Total)$	= total fugacity capacity for cell <i>i</i> , mol/m ³ [sending cell <i>i</i>]-Pa
$V_i(Total)$	= total volume of cell <i>i</i> (sum of volumes of each phase in cell), m ³ [cell <i>i</i>]

Applying this shows that the fugacity-based form for the transition probability for advective flux is:

$$T_{i \rightarrow j}^{adv}(phase) = \frac{Q(phase) \times Z_i(phase)}{V_i(Total) \times Z_i(Total)}$$

$$= \frac{v(phase) \times A_{ij} \times Z_i(phase)}{V_i(Total) \times Z_i(Total)}$$

In most applications, the volumetric flow rate $Q(phase)$ of the phase is calculated as the product of a relevant area (A_{ij}) and the volumetric flow rate per unit area, or a flow velocity (v_{ij}). Usually the relevant area is the interfacial area between the sending and receiving cells, but this is not always the case; e.g., erosion from surface soil to surface water is usually reported in units of mass[soil]/area[soil layer]-time, in which case the relevant area is the area of the surface soil layer. Table B-1 summarizes the implementation of all volumetric flows for domains in P4. These flows are discussed in more detail in the sections describing the specific domains.

B.4 Diffusive Processes

The net flux from diffusion from one cell to another cell depends on the difference in the concentrations in the two cells. This means that the direction of flux is not necessarily constant with time. However, it is possible to derive the general form for diffusion from one cell to another and then break up defining net diffusion into a part proportional to the mass in one cell and a part proportional to the mass in another cell. Although it is not known

beforehand which is the “sending” cell, if one is dealing with a fixed cell, then these terms take the mathematical form of a “sending” component to the other cell and a “receiving” component from the other cell.

In all cases, diffusion across compartment boundaries is modeled in P4 as a two-resistance model through the boundary layers on either side of the domain interface (as discussed in CalTOX, Vol. II, pp 36-41). This is first done in a general manner that simplifies the presentation, as characterization of diffusion between two cells reduces to specifying an interfacial area between the two cells and specifying the algorithm for calculating the mass transfer coefficient for a particular domain.

In the two-resistance model for molecular and turbulent diffusion, the mass transfer between a cell i to cell j depends on mass transfer through two distinct layers: the boundary in cell i and the boundary in cell j . It is assumed that the net flux is equal on both sides of the boundary between the two cells. This flux is assumed to be proportional to the difference in the bulk concentration in the cell and the concentration at the cell-side of the boundary. The constant of proportionality has units of m/day , and is called the mass transfer coefficient. Determination of the mass transfer coefficient depends on the domain type that the cell is, and in some cases on the domain type of both cells.

The general form for the net diffusive flux between two cells is given by:

$$\text{Net diffusive flux between cell } i \text{ and cell } j = F_{ij} = A_{ij} \begin{cases} U_{ij} (C_i^b - C_i^*) \\ U_{ji} (C_j^* - C_j^b) \end{cases}$$

Table B-1

Summary of Volumetric Advective Flow Velocities Considered in Prototype 4

Source/ Sending Cell	Receiving Cell	Moving Phase	Description of Phase Velocity	Units	Calculated or Specified in Prototype 4
Soil	Soil	Liquid	Precipitation driven percolation	m ³ [water]/day	Specified = A*Darcy_Liq where: A = Area of soil-soil interface, m ² Darcy_Liq = Darcy velocity of water in sending soil cell, m ³ [water]/m ² [area]- day.
		Gas	Gas Discharge	m ³ [gas]/day	Specified = A*Darcy_Gas where: A = Area of soil-soil interface, m ² Darcy_Gas = Darcy velocity of gas in sending soil cell, m ³ [gas]/m ² [area]- day.
	Air	Solid	Resuspension	m ³ [soil]/day	It is assumed that volumetric flow of particles from soil is the same as that to soil. Volumetric resuspension rate is then = Vol. Flow TO soil = A*v _d * ρ _A / ρ _P where: A = Area of soil-soil interface, m ² [area] v _d = Dry deposition velocity of particles, m/day ρ _A = Atmospheric dust load in air domain (concentration of dust in air), kg[particles]/m ³ [atmosphere] ρ _P = Density of air particles, kg[particles]/m ³ [particles]

Table B-1

Summary of Volumetric Advective Flow Velocities Considered in Prototype 4

Source/ Sending Cell	Receiving Cell	Moving Phase	Description of Phase Velocity	Units	Calculated or Specified in Prototype 4
Soil/Groundwater	Surface Water	Solid	Erosion	m ³ [soil]/day	Calculated from mass-based areal erosion rate and soil density: $= A * E / \rho_s$ where: A = Area of soil layer, m ² E = erosion rate to surface water, kg [soil]/m ² [area]-day ρ_s = density of eroding soil, kg[soil]/m ³ [soil]
Soil/Groundwater	Surface Water	Liquid	Runoff	m ³ [water]/day	= A * Runoff where: A = Area of soil layer, m ² Runoff = Amount of runoff that reaches waterbody per units area of watershed, m ³ [water]/m ² [area]-day
			Recharge	m ³ [water]/day	= A * Recharge where: A = Area of soil-surface water interface, m ² Recharge = Volume of water flow per unit area of interface, m ³ [water]/m ² [area]-day
Air	Soil and Surface Water	Solid	Wet & Dry deposition of particles	m ³ [particles]/day	Calculated: $= A * v_d * \rho_A / \rho_p$ where: A = Area of soil layer, m ² v_d = Dry deposition velocity of particles, m/day ρ_A = Atmospheric dust load in air domain (concentration of dust in air), kg[particles]/m ³ [atmosphere] ρ_p = Density of air particles, kg[particles]/m ³ [particles]
		Liquid (Vapor?)	Wet deposition of liquid		Not implemented

Table B-1

Summary of Volumetric Advective Flow Velocities Considered in Prototype 4

Source/ Sending Cell	Receiving Cell	Moving Phase	Description of Phase Velocity	Units	Calculated or Specified in Prototype 4
	Air or Air Advection Sink	Total	Wind advection	m ³ [air]/day	= A*u where: A = Area of air-air interface, m ² u = Wind velocity from sending to receiving air cell, m/day
Air	Plant Leaf	Solid	Wet deposition of particles	m ³ [particles]/day	Calculated: =A*I* (w _d * ρ _A / ρ _P) * f _L where: A = Area of soil layer containing plant I = Interception fraction (see Section 7 for description of algorithm) v _d = Deposition velocity of particles, m/day ρ _A = Atmospheric dust load in air domain (concentration of dust in air), kg[particles]/m ³ [atmosphere] ρ _P = Density of air particles, kg[particles]/m ³ [particles] f _L = Fraction of deposition adhering that is taken up by plant
Surface Water	Sediment	Solid	Sediment deposition	m ³ [suspended sediment]/day	Calculated: = A*S _{dep} / ρ _{ss} where A = Area of surface water-sediment interface, m ² S _{dep} = Deposition rate of suspended sediment to sediment bed, kg[suspended sediment]/m ² [area]-day ρ _{ss} = Density of suspended sediment, kg[suspended sediment]/m ³ [suspended sediment]
	River to river	Total	River flow	m ³ [air]/day	= A*ur where: A = Area of river parcel interface, m ² ur = River velocity from sending to receiving river cell, m/day

Table B-1

Summary of Volumetric Advective Flow Velocities Considered in Prototype 4

Source/ Sending Cell	Receiving Cell	Moving Phase	Description of Phase Velocity	Units	Calculated or Specified in Prototype 4
	Surface water advection sink	Total	Outflow	m ³ [water column]/day	<p>Calculated so that net flux of water into surface water is 0: $= (\text{Runoff} * A_{\text{SSoil}} + \text{Recharge} * A_{\text{SW-GW}} + \text{Inflow}) + (\text{Rain} - \text{EV}) * A$</p> <p>where: A = Area of surface water, m² Runoff = runoff from surface soil, m³[water reaching surface water]/m²[surface soil area]-day A_{SSoil} = Area of surface soil, m²[surface soil area] Recharge = Recharge from groundwater to surface water, m³[water]/m²[interface]-day A_{SW-GW} = Area of surface water-ground water interface, m²[interface] Rain = Precipitation rate, m³[water]/m²[surface water area]-day EV = Evaporation rate, m³[water]/m²[surface water area]-day Inflow = inflow of water to water body cell, m³[water]/day</p>
Sediment	Surface Water	Solid	Sediment resuspension	m ³ [benthic sediment]/day	<p>Calculated: $= A * S_{\text{resusp}} / \rho_{\text{bs}}$</p> <p>where: A = Area of sediment-surface water interface, m² S_{resusp} = Resuspension rate of benthic sediment to water column, kg[benthic sediment]/m²[area]-day ρ_{bs} = Density of benthic sediment, kg[benthic sediment]/m³[benthic sediment]</p>

Table B-1

Summary of Volumetric Advective Flow Velocities Considered in Prototype 4

Source/ Sending Cell	Receiving Cell	Moving Phase	Description of Phase Velocity	Units	Calculated or Specified in Prototype 4
	Sediment burial sink	Solid	Sediment burial	m ³ [sediment]/day	<p>Calculated so that amount of sediment buried is equal to maximum of 0 and amount deposited minus amount resuspended: $= A * \max\{0, S_{dep}/\rho_{ss} - S_{resusp}/\rho_{bs}\}$ where: A = Area of sediment-surface water interface, m² S_{dep} = Deposition rate of suspended sediment to sediment bed, kg[suspended sediment]/m²[area]-day ρ_{ss} = Density of suspended sediment, kg[suspended sediment]/m³[suspended sediment] S_{resusp} = Resuspension rate of benthic sediment to water column, kg[benthic sediment]/m²[area]-day ρ_{bs} = Density of benthic sediment, kg[benthic sediment]/m³[benthic sediment]</p>

where:

- F_{ij} = net diffusive flux from cell i to cell j , mol/day
 A_{ij} = interfacial area between cells i and j through which diffusion occurs, m^2
 U_{ij} = mass transfer coefficient for combined turbulent and molecular diffusion on “i” side of boundary between cells i and j , m/day (= { mol/m²[area]-day } / { mol/m³[cell i] })
 U_{ji} = mass transfer coefficient for combined turbulent and molecular diffusion on “j” side of boundary between cells i and j , m/day (= { mol/m²[area]-day } / { mol/m³[cell j] })
 C_i^{total} = total concentration of chemical in cell i , mol/m³[cell i]
 C_i^* = total concentration of chemical in cell i at the boundary with cell j but in cell i , mol/m³[cell i]
 C_j^{total} = total concentration of chemical in cell j , mol/m³[cell j]
 C_j^* = total concentration of chemical in cell j at the boundary with cell i but in cell j , mol/m³[cell j]

In order to derive the general form for diffusion, the concept of fugacity is applied. Dividing the first equation by Z_i^{total} and the second by Z_j^{total} yields:

$$\frac{C_i^*}{Z_i^{total}} = \frac{F_{ij}}{A_{ij} U_{ij} Z_i^{total}} + C_i^{total}$$

$$\frac{C_j^*}{Z_j^{total}} = \frac{F_{ij}}{A_{ij} U_{ji} Z_j^{total}} + C_j^{total}$$

If it is assumed that, at the boundary between the cells, the fugacities on both sides of the boundary are equal; i.e., if $f_i^* = C_i^*/Z_i^{total} = C_j^*/Z_j^{total} = f_j^*$, where f^* is the fugacity of a cell, then:

$$\frac{F_{ij}}{A_{ij} U_{ij} Z_i^{total}} + C_i^{total} = \frac{F_{ij}}{A_{ij} U_{ji} Z_j^{total}} + C_j^{total}$$

Solving for F_{ij} shows that:

$$F_{ij} = \left(\frac{C_i^{total}}{Z_i^{total}} - \frac{C_j^{total}}{Z_j^{total}} \right) \left(\frac{1}{A_{ij} Z_i^{total} U_{ij}} + \frac{1}{A_{ij} Z_j^{total} U_{ji}} \right)^{-1}$$

$$= \left(\frac{N_i}{Z_i V_i} - \frac{N_j}{Z_j V_j} \right) \left(\frac{1}{A_{ij} Z_i^{total} U_{ij}} + \frac{1}{A_{ij} Z_j^{total} U_{ji}} \right)^{-1}$$

where:

$$\begin{aligned}
 F_{ij} &= \text{net diffusive flux from cell } i \text{ to cell } j, \text{ mol/day} \\
 U_{ij} &= \text{mass transfer coefficient for combined turbulent and molecular diffusion on "i" side of} \\
 &\quad \text{boundary between cells } i \text{ and } j, \text{ m/day (=\{ mol/m}^2[\text{area}]\text{-day} \} \\
 &\quad \text{/\{ mol/m}^3[\text{cell } i]\})} \\
 U_{ji} &= \text{mass transfer coefficient for combined turbulent and molecular diffusion on "j" side of} \\
 &\quad \text{boundary between cells } i \text{ and } j, \text{ m/day (=\{ mol/m}^2[\text{area}]\text{-day} \} \\
 &\quad \text{/\{ mol/m}^3[\text{cell } j]\})} \\
 N_i &= \text{amount of chemical in cell } i, \text{ moles chemical} \\
 V_i &= \text{total volume of cell } i, \text{ m}^3[\text{cell } i] \\
 Z_i^{total} &= \text{total fugacity capacity for cell } i, \text{ moles chemical/m}^3[\text{cell } i]\text{-Pa}
 \end{aligned}$$

The general form for the transfer factors can now be derived. In particular, the differential equations for the amount of chemical in cells i and j are:

$$\begin{aligned}
 \frac{dN_i}{dt} &= \left(\frac{N_j}{Z_j^{total} V_j} - \frac{N_i}{Z_i^{total} V_i} \right) Y(i,j) A_{ij} + \text{other gains and losses} \\
 \frac{dN_j}{dt} &= \left(\frac{N_i}{Z_i^{total} V_i} - \frac{N_j}{Z_j^{total} V_j} \right) Y(i,j) A_{ij} + \text{other gains and losses}
 \end{aligned}$$

where $Y(i,j)=Y(j,i) = \left(\frac{1}{Z_i U_{i-j}} + \frac{1}{Z_j U_{j-i}} \right)^{-1}$. Rearranging shows that:

$$\begin{aligned}
 \frac{dN_i}{dt} &= N_j \frac{Y(i,j) A_{ij}}{Z_j^{total} V_j} - N_i \frac{Y(i,j) A_{ij}}{Z_i^{total} V_i} + \text{other gains and losses} \\
 \frac{dN_j}{dt} &= N_i \frac{Y(i,j) A_{ij}}{Z_i^{total} V_i} - N_j \frac{Y(i,j) A_{ij}}{Z_j^{total} V_j} + \text{other gains and losses}
 \end{aligned}$$

From these equations we see that the general form for the transition probability for diffusive transport from cell i to cell j is:

$$\begin{aligned}
 T_{ij}^{diff} &= \frac{Y(i,j) A_{ij}}{Z_i^{total} V_i} \\
 &= \frac{A_{ij}}{\left(\frac{1}{Z_i^{total} U_{ij}} + \frac{1}{Z_j^{total} U_{ji}} \right) Z_i^{total} V_i}
 \end{aligned}$$

where:

$$\begin{aligned} T_{ij}^{diff} &= \text{transition probability for diffusive transport from cell } i \text{ to cell } j, / \text{day} \\ U_{ij} &= \text{mass transfer coefficient for combined turbulent and molecular diffusion on "i" side of} \\ &\quad \text{boundary between cells } i \text{ and } j, \text{ m/day (=\{ mol/m}^2[\text{area}]\text{-day} \} \\ &\quad \text{/\{ mol/m}^3[\text{cell } i]\}) \\ U_{ji} &= \text{mass transfer coefficient for combined turbulent and molecular diffusion on "j" side of} \\ &\quad \text{boundary between cells } i \text{ and } j, \text{ m/day (=\{ mol/m}^2[\text{area}]\text{-day} \} \\ &\quad \text{/\{ mol/m}^3[\text{cell } j]\}) \\ V_i &= \text{total volume of cell } i, \text{ m}^3[\text{cell } i] \\ Z_i^{total} &= \text{total fugacity capacity for cell } i, \text{ moles chemical/m}^3[\text{cell } i]\text{-Pa} \end{aligned}$$

This general form is used to model diffusive transport in P4. All that must be determined for each such diffusive link between cells are the mass transfer coefficients and the interfacial area between the cells through which diffusion occurs.

Table B-2 summarizes how the mass transfer coefficients are estimated for all diffusive transfers considered in P4. These are discussed in more detail in the sections describing the specific domains.

B.5 Reaction and Transformation Processes

In P4, reaction and transformation processes are modeled using either a specified reaction/ transformation rate or chemical half-life for each cell. In all cases, the mass of chemical transformed in a given cell is assumed to be lost from the system into a sink cell which receives input only from the particular cell. For a given cell i and an associated sink, the transition probability T_i^{sink} that represents the transformation/reaction process is simply the specified or calculated reaction/ transformation rate.

Table B-2

Summary of Diffusion Mass Transfer Coefficients Considered in Prototype 4

Sending Cell	Receiving Cell	$U_{\text{sending} \rightarrow \text{Receiving}}$ (Mass transfer coefficient, m/day)	Reference
Air	Surface Water	$= D_{\text{air}}^{\text{eff}} / \delta_{\text{aw}}$ $= 0.00316 * \text{WindSpeed} * (18/\text{MW})^{1/2}$, if WindSpeed > 0.5 m/s ¹ $= 0.00162 * \text{WindSpeed} * (18/\text{MW})^{1/2}$, if WindSpeed < 0.5 m/s where: $D_{\text{air}}^{\text{eff}} = (Z_{\text{air}}/Z_{\text{total air1}})(D_{\text{air}})$ D_{air} = Chemical diffusivity in air, m ² /day δ_{aw} = Boundary layer thickness in air above surface water, m Windspeed = Wind speed, m/day MW = Molecular weight of chemical, g/mol	Southworth (1979) See p. 42 of CalTox manual
Surface Water	Air	Specified (0.24 m ² /s)	CalTox p. 41
Air	Soil	$= D_{\text{air}}^{\text{eff}} / \delta_{\text{as}}$ where: $D_{\text{air}}^{\text{eff}} = (Z_{\text{air}}/Z_{\text{total air2}})(D_{\text{air}})$ D_{air} = Chemical diffusivity in air, m ² /day (Specified) δ_{as} = Boundary layer thickness in air above soil, m (Specified)	

¹The general form of this equation includes a term for the velocity of the surface water. In Prototype 2.0 we are assuming that this velocity is 0.

²This is also based on a slow current velocity.

Table B-2

Summary of Diffusion Mass Transfer Coefficients Considered in Prototype 4.0

Sending Cell	Receiving Cell	$U_{\text{sending} \rightarrow \text{Receiving}}$ (Mass transfer coefficient, m/day)	Reference
Soil	Air	$= D_{\text{eff}} / \delta_{\text{sa}}$ <p>where:</p> $D_{\text{eff}} = \text{Effective diffusivity in soil, m}^2/\text{day}$ $= Z_{\text{water}}/Z_{\text{total}})D_{\text{water}} \theta^{10/3} / \phi^2 +$ $(Z_{\text{air}}/Z_{\text{total}})D_{\text{air}} \epsilon^{10/3} / \phi^2$ <p>where:</p> $Z_{\text{water}} = \text{Fugacity capacity for water, mol/m}^3\text{-Pa}$ $Z_{\text{air}} = \text{Fugacity capacity in air, mol/m}^3\text{-Pa}$ $Z_{\text{total}} = \text{Total fugacity capacity for sending soil layer, mol/m}^3\text{-Pa}$ $D_{\text{water}} = \text{Diffusion coefficient in pure water, m}^2/\text{day}$ $D_{\text{air}} = \text{Diffusion coefficient in pure air, m}^2/\text{day}$ $\theta = \text{Volume fraction of water in sending soil layer, m}^3[\text{water}]/\text{m}^3[\text{soil layer}]$ $\epsilon = \text{Volume fraction of air in sending soil layer, m}^3[\text{air}]/\text{m}^3[\text{soil layer}]$ $\phi = \text{Total void fraction in sending soil layer, } \phi = \theta + \epsilon$ δ_{sa} <p>= Boundary layer thickness in sending soil with air, m.</p> $= 0.108 * D_{\text{eff (ss)}}^{0.229} \text{ (for surface soil)}$ $= 318.4 * D_{\text{eff (rz)}}^{0.683} \text{ (for root zone)}$ $= \text{Depth of layer} / 2 \text{ (for vadose zones 1 and 2)}$	CalTox vol. II, p.35-36, based on Jury et al. (1983)
Soil	Soil	Same as for Soil -> Air	CalTox
Surface Water	Sediment	$= D_{\text{water}}^{\text{eff}} / \delta_{\text{wd}}$ <p>where:</p> $D_{\text{water}}^{\text{eff}} = (Z_{\text{water}}/Z_{\text{total surface water}}) D_{\text{water}}$ $D_{\text{water}} = \text{Diffusion coefficient in water, m}^2/\text{day}$ $\delta_{\text{wd}} = \text{Boundary layer thickness in surface water above sediment, m. Specified.}$	CalTox, p.36, based on Jury et al. (1983).

Table B-2

Summary of Diffusion Mass Transfer Coefficients Considered in Prototype 4.0

Sending Cell	Receiving Cell	$U_{\text{sending} \rightarrow \text{Receiving}}$ (Mass transfer coefficient, m/day)	Reference
Sediment	Surface water	$= D_{\text{eff}} / \delta_{\text{dw}}$ <p>where:</p> $D_{\text{eff}} = \text{Effective diffusivity in sediment, m}^2/\text{day}$ $= (Z_{\text{water}}/Z_{\text{total}}) D_{\text{water}} \phi^{4/3}$ <p>where:</p> $Z_{\text{water}} = \text{Fugacity capacity for water, mol/m}^3\text{-Pa}$ $Z_{\text{total}} = \text{Total fugacity capacity for sediment layer, mol/m}^3\text{-Pa}$ $D_{\text{water}} = \text{Diffusion coefficient in pure water, m}^2/\text{day}$ $\phi = \text{Volumetric pore space filled with water in sediment layer, m}^3[\text{water}]/\text{m}^3[\text{sediment layer}]$ δ_{dw} $= \text{Boundary layer thickness in sediment below surface water, m}$ $= 318 D_{\text{eff}}^{0.683}$	<p>CalTox, p.36, based on Jury et al. (1983).</p> <p>CalTox, p. 44, Eq. 58 (based on Jury et al. 1983)</p>

APPENDIX C

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